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On the Randić Index of Unicyclic Graphs with Fixed Diameter

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Abstract

The Randić index $R(G)$ of a graph G is the sum of the weights $\frac{1}{\sqrt{d(u)d(v)}}$ of all edges uv of G, where $d(u)$ denotes the degree of the vertex u. In this paper, we give sharp lower bounds of Randić index of unicyclic graphs with n vertices and diameter d, which partly confirms a conjecture in [1](MATCH Commun. Math. Comput. Chem. 58(2007) 83-102) by Aouchiche, Hansen and Zheng.

1. Introduction

The Randić index of an organic molecule whose molecular graph is G is defined in [27] as

$$R(G) = \sum_{u,v} \frac{1}{\sqrt{d(u)d(v)}},$$

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where $d(u)$ denotes the degree of the vertex u of G and the summation goes over all pairs of adjacent vertices of G. The research background of Randić index together with its generalization appears in chemistry or mathematical chemistry and can be found in the literature (see [11]-[13]).

First we introduce some graph notations used in this paper. We only consider finite, undirected and simple graphs. Other undefined terminologies and notations may refer to [3]. For a vertex x of a graph G, we denote the neighborhood and the degree of x by $N(x)$ and $d(x)$, respectively. Let $S \subseteq V(G)$, we will use $G - S$ to denote the graph that arises from G by deleting the vertices in S together with their incident edges. If $S = \{v\}$, we write $G - v$ for $G - \{v\}$. We will use $G - uv$ to denote the graph that arises from G by deleting the edge $uv \in E(G)$. Similarly, $G + uv$ is a graph that arises from G by adding an edge $uv \notin E(G)$, where $u,\ v \in V(G)$. A *pendent vertex* is a vertex of degree 1. For two vertices $u, v \in V(G)$ $(u \neq v)$, the distance between u and v, denoted by $d_G(u, v)$, is the number of edges in a shortest path joining u and v in G. The diameter of a graph G, denoted by $\mathrm{diam}(G)$, is the maximum distance between any two vertices of G.

Unicyclic graphs are connected graphs with n vertices and n edges. Let $V_0 = \{v : v \text{ is a pendent vertex of } G\}$ and $V_1 = \bigcup_{v \in V_0} N(v)$.

Recently, there are many results concerning (general) Randić index of graphs (see [1], [2], [4]-[10], [14]-[26], [28]-[29]). In [1], Aouchiche, Hansen and Zheng proposed the following conjecture.

Conjecture A. *For any connected graph on $n \geq 3$ vertices with Randić index R and diameter d,*

$$R - d \geq \sqrt{2} - \tfrac{n+1}{2} \qquad \textit{and} \qquad \tfrac{R}{d} \geq \tfrac{n-3+2\sqrt{2}}{2n-2},$$

with equality if and only if G is the path P_n.

Li and Zhao [17] considered the relation between the Randić index and the diameter of trees and given the following result.

Theorem B ([17]). *Let T be a tree of order n with diameter $d \geq 3$, then*

$$R(T) \geq \frac{n - d + \frac{1}{\sqrt{2}}}{\sqrt{n - d + 1}} + \frac{d - 3 + \sqrt{2}}{2} \tag{1}$$

and equality in (1) if and only if $T \cong S^*_{n,d}$, where $S^*_{n,d}$ be a tree of order n obtained from a star S_{n-d+1} by attaching a path of order $d - 1$ to the center of S_{n-d+1}.

If $\mathrm{diam}(T) = 2$ for a tree T of order $n \geq 3$, then $T \cong S_n$, and then

$$R(T) - 2 = \sqrt{n-2} - 2 \geq \sqrt{2} - \frac{n+1}{2}, \quad \frac{R(T)}{2} = \frac{\sqrt{n-1}}{2} \geq \frac{n-3+2\sqrt{2}}{2n-2}$$

and equality holds if and only if $n = 3$, i.e., $T \cong P_3$. Let $F(d) = \frac{n-d+\frac{1}{\sqrt{2}}}{\sqrt{n-d+1}} + \frac{d-3+\sqrt{2}}{2}$, $d \geq 3$. Then

$$\frac{F(d)}{d} - \frac{1}{2} = \frac{n-d+\frac{1}{\sqrt{2}}}{d\sqrt{n-d+1}} - \frac{3-\sqrt{2}}{2d} \geq \frac{1+\frac{1}{\sqrt{2}}}{d\sqrt{2}} - \frac{3-\sqrt{2}}{2d} = \frac{\sqrt{2}-1}{d} > 0.$$

Note that

$$\begin{aligned} \frac{\partial(F(d)-d)}{\partial d} &= -\frac{1}{2}(n-d+1)^{-\frac{3}{2}}\left(n-d+2-\frac{1}{\sqrt{2}}\right) - \frac{1}{2} < 0, \\ \frac{\partial(\frac{F(d)}{d})}{\partial d} &= \frac{1}{d}\left[-\frac{1}{2}(n-d+1)^{-\frac{3}{2}}\left(n-d+2-\frac{1}{\sqrt{2}}\right) + \frac{1}{2} - \frac{F(d)}{d}\right] < 0. \end{aligned}$$

Hence by (1), we have

$$\begin{aligned} R(T) - d &\geq F(d) - d \geq F(n-1) - (n-1) = \sqrt{2} - \frac{n+1}{2}, \\ \frac{R(T)}{d} &\geq \frac{F(d)}{d} \geq \frac{F(n-1)}{n-1} = \frac{n-3+2\sqrt{2}}{2n-2}. \end{aligned}$$

Moreover, the equalities hold if and only if $d = n-1$, that is, G is the path P_n.

Note C. *The Conjecture A is true for trees.*

In the following, we will show that the Conjecture A is true for unicyclic graphs. Let $\mathscr{U}_{n,d} = \{G : G \text{ is a unicyclic graph with } n \text{ vertices and diameter } d\}$, where $1 \leq d \leq n-2$. Then $\mathscr{U}_{n,1} = \{C_3\}$ and $\mathscr{U}_{n,2} = \{U_n^*, C_4, C_5\}$, where $n \geq 4$ and U_n^* is the graph obtained from star S_n by adding a new edge between its two pendent vertices. It is easy to check $R(C_n) \geq R(U_n^*)$.

Denote

$$\varphi(n,d) = \begin{cases} \frac{n-4+\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{3}}}{\sqrt{n-2}} + \frac{1+\sqrt{2}}{\sqrt{6}}, & d = 3, \\ \frac{n-5+\sqrt{2}}{\sqrt{n-3}} + \frac{1+\sqrt{2}}{\sqrt{3}}, & d = 4, \\ \frac{n-d-1+\sqrt{2}}{\sqrt{n-d+1}} + \frac{d-5}{2} + \frac{1+\sqrt{3}}{\sqrt{2}}, & d \geq 5. \end{cases}$$

In this paper, we mainly show the the following theorem in Section 2, which partly confirms Conjecture A.

Theorem D. *Let $G \in \mathscr{U}_{n,d}$, $3 \le d \le n-2$. Then*

$$R(G) \ge \varphi(n,d) \tag{2}$$

and equality in (2) holds if and only if $G \cong U_n^d$, where U_n^d are shown in Fig. 1.

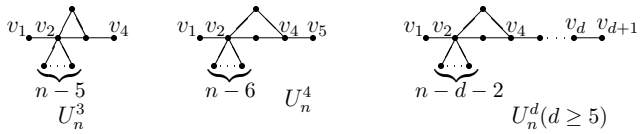


Fig. 1

Denote $\phi(n) = \sqrt{2} - \frac{n+1}{2}$ and $\psi(n) = \frac{n-3+2\sqrt{2}}{2n-2}$, where $n \ge 3$. Then

$$\begin{aligned}
(R(C_3)-1)-\phi(3) &= \frac{5}{2}-\sqrt{2}>0, \qquad \frac{R(C_3)}{1}-\psi(3)=\frac{3-\sqrt{2}}{2}>0,\\
R(U_n^*)-2-\phi(n) &= \frac{n-3+\sqrt{2}}{\sqrt{n-1}}+\frac{1}{2}-2-\sqrt{2}+\frac{n+1}{2}>0 \ \text{ for } n\ge 4,\\
\frac{R(U_n^*)}{2}-\psi(n) &= \frac{n-3+\sqrt{2}}{2\sqrt{n-1}}+\frac{1}{4}-\frac{n-3+2\sqrt{2}}{2n-2}>0 \ \text{ for } n\ge 4,\\
\varphi(n,3)-3-\phi(n) &= \frac{n-4+\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{3}}}{\sqrt{n-2}}+\frac{n-5}{2}+\frac{1+\sqrt{2}-2\sqrt{3}}{\sqrt{6}}>0 \text{ for } n\ge 5,\\
\frac{\varphi(n,3)}{3}-\psi(n) &= \frac{n-4+\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{3}}}{3\sqrt{n-2}}-\frac{n-3+2\sqrt{2}}{2n-2}+\frac{1+\sqrt{2}}{3\sqrt{6}}>0 \text{ for } n\ge 5,\\
\varphi(n,4)-4-\phi(n) &= \frac{n-5+\sqrt{2}}{\sqrt{n-3}}+\frac{n-7}{2}+\frac{2+\sqrt{2}-\sqrt{12}}{\sqrt{6}}>0 \text{ for } n\ge 6,\\
\frac{\varphi(n,4)}{4}-\psi(n) &= \frac{n-4+\sqrt{2}}{4\sqrt{n-3}}-\frac{n-3+2\sqrt{2}}{2n-2}+\frac{2+\sqrt{2}}{4\sqrt{6}}>0 \text{ for } n\ge 6.
\end{aligned}$$

Note that, for $d \ge 5$, $\frac{\varphi(n,d)}{d}-\frac{1}{2}=\frac{n-d-1+\sqrt{2}}{d\sqrt{n-d+1}}+\frac{\sqrt{6}+\sqrt{2}-5}{2d} \ge \frac{2+\sqrt{2}}{d\sqrt{3}}-\frac{\sqrt{6}+\sqrt{2}}{2d}>0$. Hence

$$\begin{aligned}
\frac{\partial(\varphi(n,d)-d)}{\partial d} &= -\frac{1}{2}(n-d+1)^{-\frac{1}{2}}-\frac{1}{2}\left(2-\sqrt{2}\right)(n-d+1)^{-\frac{3}{2}}-\frac{1}{2}<0,\\
\frac{\partial(\frac{\varphi(n,d)}{d})}{\partial d} &= \frac{1}{d}\left[-\frac{1}{2}(n-d+1)^{-\frac{3}{2}}\left(n-d+3-\sqrt{2}\right)+\frac{1}{2}-\frac{\varphi(n,d)}{d}\right]<0.
\end{aligned}$$

Thus by (2),

$$R(G)-d \ge \varphi(n,d)-d \ge \varphi(n,n-2)-(n-2)=\frac{5+\sqrt{3}+\sqrt{2}}{\sqrt{6}}-\frac{n+3}{2}>\phi(n),$$

$$\frac{R(G)}{d} \geq \frac{\varphi(n,d)}{d} \geq \frac{\varphi(n,n-2)}{n-2} = \frac{\frac{5+\sqrt{2}+\sqrt{3}}{\sqrt{6}} + \frac{n-7}{2}}{n-2} > \frac{n-3+2\sqrt{2}}{2n-2} = \psi(n).$$

Note E. *The Conjecture A is true for unicyclic graphs.*

2. Proof of Theorem D

We first give some lemmas that will be used in the proof of our result.

Lemma 1. *(i) Let* $f(x) = \frac{x+\sqrt{2}-2}{\sqrt{x}}$ *and* $g(x) = \frac{x-2+\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{3}}}{\sqrt{x}}$, *where* $x \geq 3$. *Then both* $f(x) - f(x+1)$ *and* $g(x-1) - g(x)$ *are strictly monotone increasing in* $x \geq 3$;

(ii) Let $h_1(x) = \frac{x}{2} - \frac{x+x_0}{\sqrt{x}}$ *and* $h_2(x) = \frac{x-2+k_0}{\sqrt{x-1}} - \frac{x-2+l_0}{\sqrt{x}}$, *where* $x_0 > 3(\sqrt{3}-1)$, $k_0 \leq \frac{1}{\sqrt{2}}$ *and* $l_0 \geq \sqrt{2}$ *are three constant numbers. Then* $h_1(x)$ *and* $h_2(x)$ *are strictly monotone increasing in* $x \geq 3$;

Proof. (i) Follows from, for $x \geq 3$,

$$\frac{d^2 f(x)}{dx^2} = \frac{-x^{-\frac{5}{2}}(x+6-3\sqrt{2})}{4} < 0, \quad \frac{d^2 g(x)}{dx^2} = \frac{-x^{-\frac{5}{2}}(x+6-\frac{3}{\sqrt{2}}-\frac{3}{\sqrt{3}})}{4} < 0.$$

(ii) Note that, for $x \geq 3$,

$$\begin{aligned}
\frac{dh_1(x)}{dx} &= \frac{1}{2}x^{-\frac{3}{2}}\left(x\sqrt{x} - x + x_0\right) > 0; \\
\frac{dh_2(x)}{dx} &= \frac{1}{2}\left[(x-1)^{-\frac{1}{2}} - x^{-\frac{1}{2}}\right] + \frac{1-k_0}{2}(x-1)^{-\frac{3}{2}} - \frac{2-l_0}{2}x^{-\frac{3}{2}} \\
&= \frac{1}{4}\zeta^{-\frac{3}{2}} + \frac{1-k_0}{2}(x-1)^{-\frac{3}{2}} - \frac{2-l_0}{2}x^{-\frac{3}{2}} \\
&> \frac{1}{4}x^{-\frac{3}{2}} + \frac{1-k_0}{2}x^{-\frac{3}{2}} - \frac{2-l_0}{2}x^{-\frac{3}{2}} = \frac{2l_0-1-2k_0}{4}x^{-\frac{3}{2}} > 0,
\end{aligned}$$

where $\zeta \in (x-1, x)$. Hence (ii) follows. ■

Lemma 2. *(i) For* $d = 4$ *and* $n \geq d+2 \geq 6$, *and* $d \geq 5$ *and* $n \geq d+3 \geq 7$, $\frac{n-6}{2} + \frac{2\sqrt{2}+2}{\sqrt{3}} \geq \varphi(n,d)$ *and equality holds if and only if* $d = 4$ *and* $n = 6$;

(ii) For $d \geq 5$ *and* $n \geq d+2$, $\frac{n-7}{2} + \frac{5+\sqrt{3}+\sqrt{2}}{\sqrt{6}} \geq \varphi(n,d)$ *and equality holds if and only if* $n = d+2 \geq 7$.

Proof. (i) Let $h_1(x) = \frac{x}{2} - \frac{x+\sqrt{2}-2}{\sqrt{x}}$. Then by Lemma 1(ii),

$$\frac{n-6}{2} + \frac{2\sqrt{2}+2}{\sqrt{3}} - \varphi(n,4) = h_1(n-3) + \frac{1+\sqrt{2}}{\sqrt{3}} - \frac{3}{2} \geq h_1(3) + \frac{1+\sqrt{2}}{\sqrt{3}} - \frac{3}{2} = 0;$$

and for $d \geq 5$,

$$\begin{aligned}\frac{n-6}{2}+\frac{2\sqrt{2}+2}{\sqrt{3}}-\varphi(n,d) &= h_1(n-d+1)+\frac{2}{\sqrt{3}}+\frac{1}{\sqrt{6}}-\frac{1}{\sqrt{2}}-1\\ &\geq h_1(4)\frac{2}{\sqrt{3}}+\frac{1}{\sqrt{6}}-\frac{1}{\sqrt{2}}-1>0.\end{aligned}$$

From the above arguments, the equality holds if and only if $d=4$ and $n-3=3$.

(ii) Let $h_1(x)$ defined in (i). Then

$$\begin{aligned}&\frac{n-7}{2}+\frac{5+\sqrt{3}+\sqrt{2}}{\sqrt{6}}-\varphi(n,d)\\ =\ & h_1(n-d+1)+\frac{5+\sqrt{3}+\sqrt{2}}{\sqrt{6}}-\frac{3}{2}-\frac{3}{\sqrt{6}}-\frac{1}{\sqrt{2}}\\ \geq\ & h_1(3)+\frac{2}{\sqrt{6}}+\frac{1}{\sqrt{3}}-\frac{3}{2}=0.\end{aligned}$$

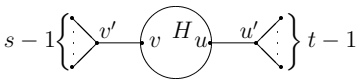
From the above arguments, the equality holds if and only if $n-d+1=3$. ■

Let H_1, H_2 be two connected graphs with $V(H_1)\cap V(H_2)=\{v\}$. Let H_1vH_2 be a graph defined by $V(G)=V(H_1)\cup V(H_2)$, $V(H_1)\cap V(H_2)=\{v\}$ and $E(G)=E(H_1)\cup E(H_2)$.

Lemma 3 [28]. *Let H be a connected graph and T_l be a tree of order l with $V(H)\cap V(T_l)=\{v\}$. Then*

$$R(HvT_l)\geq R(HvK_{1,l-1})$$

and equality holds if and only if $HvT_l\cong HvK_{1,l-1}$, where v is identified with the center of the star $K_{1,l-1}$ in $HvK_{1,l-1}$.



$G_{s,t}$

Fig. 2

Lemma 4 [17]. *Let $G_{s,t}$ be a graph shown in Fig. 2, where H is a connected graph. If $s\geq t\geq 2$ and $d_G(u)\geq d_G(v)$, then*

$$R(G_{s,t})>R(G_{s+1,t-1}).$$

Lemma 5 [7]. *Let G be a unicyclic graph of order n. Then $R(G)\leq R(C_n)$ and equality holds if and only if $G\cong C_n$.*

Let $P_{n,l}$ (see Fig. 3) be unicyclic graphs of order n obtained from a cycle C_{n-l} by attaching a path of length l ($l \geq 1$) at one vertex of C_{n-l}, and the only pendent vertex of $P_{n,l}$ is called the tail of $P_{n,l}$. Let $Q_{n,i,j}$ (see Fig. 3) be those unicyclic graphs of order n and diameter d obtained from a cycle C_{n-i-j} by attaching a path $v_1v_2\dots v_iv_{i+1}$ of length i and a path $v_{d+1-j}v_{d+2-j}\dots v_dv_{d+1}$ of length j ($i, j \geq 1$) at two vertices of the cycle, respectively. Let $R_{n,i,l}$ (see Fig. 3) be a unicyclic graph of order n and diameter d obtained from a graph $P_{n-d,l}$ by attaching a path $v_1v_2\dots v_i$ of length $i-1$ and a path $v_iv_{i+1}\dots v_{d+1}$ of length $d+1-i$ at the tail of $P_{n-d,l}$, respectively.

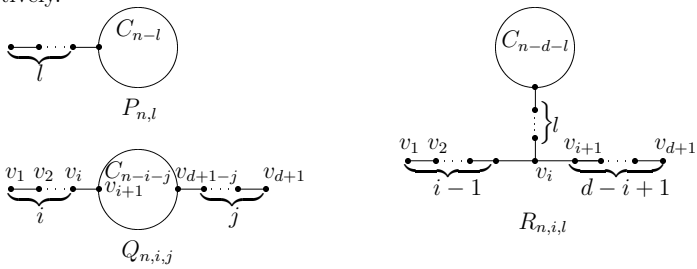


Fig. 3

Lemma 6. *Suppose that $G \in \mathscr{U}_{n,d}$ ($3 \leq d \leq n-2$) with $V_0 \neq \emptyset$. If $G - v \in \mathscr{U}_{n-1,d-1}$ for any $v \in V_0$, then*

$$R(G) \geq \varphi(n, d). \tag{3}$$

Moreover, the equality in (3) holds if and only if $d = n-2$ and $G \cong U^d_{d+2}$.

Proof. Since G is unicyclic graph and for any $v \in V_0$, $G - v \in \mathscr{U}_{n-1,d-1}$, we have $G \cong P_{n,l}$, or $G \cong Q_{n,i,j}$, or $G \cong R_{n,i,l}$.

Case 1. $G \cong P_{n,l}$.

In this case, if $d = 4$, then $n \geq 6$, and thus by Lemma 1(ii), we have

$$R(G) = \begin{cases} \frac{n-4+\sqrt{2}+\sqrt{6}}{2} = \varphi(n,4) + \frac{n-4}{2} - \frac{n-5+\sqrt{2}}{\sqrt{n-3}} + \frac{1+\sqrt{3}-\sqrt{2}}{\sqrt{6}} > \varphi(n,4), & l > 1, \\ \frac{1+\sqrt{2}}{\sqrt{3}} + \frac{n-3}{2} = \varphi(n,4) + \frac{n-3}{2} - \frac{n-5+\sqrt{2}}{\sqrt{n-3}} > \varphi(n,4), & l = 1. \end{cases}$$

If $d \geq 5$, then $n - d \geq 2$, and thus by Lemma 1(ii), we have

$$R(G) = \begin{cases} \frac{n-4+\sqrt{2}+\sqrt{6}}{2} = \varphi(n,d) + \frac{n-d+1}{2} - \frac{n-d-1+\sqrt{2}}{\sqrt{n-d+1}} > \varphi(n,d), & l > 1, \\ \frac{1+\sqrt{2}}{\sqrt{3}} + \frac{n-3}{2} = \varphi(n,d) + \frac{n-d+2}{2} - \frac{n-d-1+\sqrt{2}}{\sqrt{n-d+1}} + \frac{\sqrt{2}-\sqrt{3}-1}{\sqrt{6}} > \varphi(n,d), & l = 1. \end{cases}$$

Case 2. $G \cong Q_{n,i,j}$.

Subcase 2.1. $i+j=d$.

In this subcase, $i,j\geq 2$ by the assumption. Thus by Lemma 2,

$$R(G)=\frac{n-6+4\sqrt{2}}{2}=\left(\frac{n-6}{2}+\frac{2\sqrt{2}+2}{\sqrt{3}}\right)+2\sqrt{2}-\frac{2\sqrt{2}+2}{\sqrt{3}}>\varphi(n,d).$$

Subcase 2.2. $i+j=d-1$.

In this subcae, if $d=3$, then $G\cong U_5^3$ by the assumption, and thus the result holds. If $d\geq 4$, then by Lemma 2, we have

$$R(G)=\begin{cases}\frac{n-6+\sqrt{2}+\sqrt{6}}{2}+\frac{\sqrt{3}+1}{3}>\frac{n-6}{2}+\frac{2\sqrt{2}+2}{\sqrt{3}}\geq\varphi(n,d), & i=1;\\ \frac{n-7+2\sqrt{2}}{2}+\frac{2\sqrt{6}+1}{3}>\frac{n-7}{2}+\frac{5+\sqrt{3}+\sqrt{2}}{\sqrt{6}}\geq\varphi(n,d), & i>1.\end{cases}$$

Subcase 2.3. $i+j\leq d-2$.

In this subcase, we have $d\geq 4$, and $n-d\geq 3$ when $d\geq 5$. By Lemma 2, we have

$$R(G)=\begin{cases}\frac{n-6}{2}+\frac{2\sqrt{2}+2}{\sqrt{3}}\geq\varphi(n,d),\ i=1,j=1; & (4)\\ \frac{n-7}{2}+\frac{5+\sqrt{3}+\sqrt{2}}{\sqrt{6}}\geq\varphi(n,d),\ i=1,j>1; & (5)\\ \frac{n-8+2\sqrt{2}+2\sqrt{6}}{2}=\left(\frac{n-6}{2}+\frac{2\sqrt{2}+2}{\sqrt{3}}\right)+\left(\sqrt{2}-1\right)\left(1+\frac{2}{\sqrt{6}}\right)>\varphi(n,d),\ i,j>1. & \end{cases}$$

The equalities in (4) and (5) hold only if $G\cong U_6^4$ and $G\cong U_{d+2}^d$, respectively.

Case 3. $G\cong R_{n,p,i}$.

In this case, $i,d-i+1\geq 2$. Thus from the above calculations, we have

$$R(G)=\begin{cases}\frac{n-7+2\sqrt{2}}{2}+\frac{1+2\sqrt{6}}{3}>\varphi(n,d), & l=1,\\ \frac{n-8+2\sqrt{2}+2\sqrt{6}}{2}>\varphi(n,d), & l>1.\end{cases}$$

Therefore the proof of the theorem is complete. ■

Theorem 7. Suppose that $G\in\mathscr{U}_{n,3},\ n\geq 5$. Then

$$R(G)\geq\frac{n-4+\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{3}}}{\sqrt{n-2}}+\frac{1}{\sqrt{6}}+\frac{1}{\sqrt{3}} \tag{6}$$

and equality in (6) holds if and only if $G\cong U_n^3$.

Proof. We apply induction on n. If $n=5$, then the theorem holds by Lemma 6. So in the following proof, we assume that $n\geq 6$.

By Lemmas 5 and 6, we may assume that $V_0\neq\emptyset$ and there exists a vertex $u_0\in V_0$ such that $G-u_0$ containing a path of length 3. Let u be the neighbor vertex of u_0 in G. We consider two cases.

Case 1. $|N(u) \setminus V_0| \geq 2$.

Let $d(u) = t$. Then $3 \leq t \leq n-2$. Denote $N(u) \cap V_0 = \{v_1, \ldots, v_r\}$ and $N(u) \setminus V_0 = \{x_1, \ldots, x_{t-r}\}$. Then $r \geq 1$, $t-r = |N(u) \setminus V_0| \geq 2$ and all $d(x_i) = d_i \geq 2$. Let $G' = G - v_1$. Then $G' \in \mathscr{U}_{n-1,3}$. Note that

$$R(G) = R(G') + \frac{r}{\sqrt{t}} - \frac{r-1}{\sqrt{t-1}} + \sum_{i=1}^{t-r} \frac{1}{\sqrt{d_i}} \left(\frac{1}{\sqrt{t}} - \frac{1}{\sqrt{t-1}} \right). \tag{7}$$

Subcase 1.1 $d_i \geq 3$ *for some* i, $1 \leq i \leq t-r$.

Assume, without loss of generality, that $d_1 \geq 3$. By (7), we have

$$\begin{aligned} R(G) &\geq R(G') + \frac{r}{\sqrt{t}} - \frac{r-1}{\sqrt{t-1}} + \left(\frac{1}{\sqrt{3}} + \frac{t-r-1}{\sqrt{2}} \right) \left(\frac{1}{\sqrt{t}} - \frac{1}{\sqrt{t-1}} \right) \\ &\geq \varphi(n-1,3) + \frac{t-2+\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{3}}}{\sqrt{t}} - \frac{t-3+\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{3}}}{\sqrt{t-1}} \\ &\qquad + (t-r-2)\left(\frac{1}{\sqrt{2}} - 1\right)\left(\frac{1}{\sqrt{t}} - \frac{1}{\sqrt{t-1}}\right) \\ &\geq \varphi(n,3) + \frac{n-5+\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{3}}}{\sqrt{n-3}} - \frac{n-4+\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{3}}}{\sqrt{n-2}} \\ &\qquad + \frac{t-2+\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{3}}}{\sqrt{t}} - \frac{t-3+\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{3}}}{\sqrt{t-1}}. \qquad (8) \\ &\geq \varphi(n,3) + [g(n-3) - g(n-2)] - [g(t-1) - g(t)] \geq \varphi(n,3), \end{aligned}$$

where $g(x) = \frac{x-2+\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{3}}}{\sqrt{x}}$. The last inequality follows by Lemma 1(i) as $t \leq n-2$.

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

$$R(G') = \varphi(n-1,3), \;\; t = n-2, \;\; t-r = 2 \;\; \text{and} \;\; d_1 = 3, \; d_2 = 2.$$

By the induction hypothesis, $G' \cong U^3_{n-1}$. Hence $G \cong U^3_n$ and it is easy to check $R(U^3_n) = \varphi(n,3)$. ■

Subcase 1.2 $d_i = 2$ for all i.

In this subcase, $G' \ncong U^3_{n-1}$. Then $R(G') > \varphi(n-1,3)$ by the induction hypothesis. By (7), we have

$$R(G) \geq R(G') + \frac{r}{\sqrt{t}} - \frac{r-1}{\sqrt{t-1}} + \frac{t-r}{\sqrt{2}} \left(\frac{1}{\sqrt{t}} - \frac{1}{\sqrt{t-1}} \right)$$

$$\begin{aligned}
&> \varphi(n-1,3)+\sqrt{t}-\sqrt{t-1}+(t-r)\left(\frac{1}{\sqrt{2}}-1\right)\left(\frac{1}{\sqrt{t}}-\frac{1}{\sqrt{t-1}}\right)\\
&\geq \varphi(n,3)+\frac{n-5+\sqrt{2}}{\sqrt{n-3}}-\frac{n-4+\sqrt{2}}{\sqrt{n-2}}+\frac{t+\sqrt{2}-2}{\sqrt{t}}-\frac{t+\sqrt{2}-3}{\sqrt{t-1}}\\
&> \varphi(n,3)+[f(n-3)-f(n-2)]-[f(t-1)-f(t)]\geq \varphi(n,3),
\end{aligned}$$

where $f(x)=\frac{x+\sqrt{2}-2}{\sqrt{x}}$ and the last inequality follows by Lemma 1(i) as $t\leq n-2$.

Case 2. $|N(u)\setminus V_0|=1$.

In this case, $G-u\cong K_3\cup(n-4)P_1$ as $d=3$. Thus we have

$$\begin{aligned}
R(G) &= \frac{n-4+\frac{1}{\sqrt{3}}}{\sqrt{n-3}}+\frac{2}{\sqrt{6}}+\frac{1}{2}\\
&= \varphi(n,3)+\frac{n-4+\frac{1}{\sqrt{3}}}{\sqrt{n-3}}-\frac{n-4+\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{3}}}{\sqrt{n-2}}+\frac{1}{\sqrt{6}}+\frac{1}{2}-\frac{1}{\sqrt{3}}>\varphi(n,3).
\end{aligned}$$

Therefore the proof of the theorem is complete. ■

Theorem 8. Suppose that $G\in\mathscr{U}_{n,d}$, $4\leq d\leq n-2$. Then

$$R(G)\geq\varphi(n,d) \tag{9}$$

and equality in (9) holds if and only if $G\cong U_n^d$.

Proof. First we note if $G\cong U_n^d$ for $d\geq 4$, then (9) holds.

Now, we choose $G\in\mathscr{U}_{n,d}$, $4\leq d\leq n-2$ such that $R(G)$ is as small as possible. Since G has a path of length d, $n\geq d+2$. For d fixed, we apply induction on n. If $n=d+2$, then the theorem holds by Lemma 6. So in the following proof, we assume $n\geq d+3$. Let $P=v_1v_2\cdots v_dv_{d+1}$ be a path of length d in G and C be the only cycle of G.

By Lemmas 5 and 6, we may assume that $V_0\neq\emptyset$ and there exists a vertex $u_0\in V_0$ such that $G-u_0$ containing a path of length d. Let V_0' denote the set of all such vertices u_0 just mentioned.

Let $u\in V_1\cap N_G(V_0')$ with $d(u)=t+1$. Then $1\leq t\leq n-d$. Denote $N(u)\cap V_0=\{w_1,\ldots,w_r\}$ and $N(u)\setminus V_0=\{x_1,\ldots,x_{t-r+1}\}$. Then all $d(x_i)=d_i\geq 2$.

Case 1. There exists some $u\in V_1\cap N_G(V_0')$ such that $|N(u)\setminus V_0|\geq 2$.

In this case, $t-r\geq 1$ and $r\geq 1$. Let $G'=G-w_1$. Then $G'\in\mathscr{U}_{n-1,d}$. Thus

$$R(G)\geq R(G')+\frac{r}{\sqrt{t+1}}-\frac{r-1}{\sqrt{t}}+\frac{t-r+1}{\sqrt{2}}\left(\frac{1}{\sqrt{t+1}}-\frac{1}{\sqrt{t}}\right)$$

$$\begin{aligned}
&\geq \varphi(n-1,d)+\sqrt{t+1}-\sqrt{t}+(t-r+1)\left(\frac{1}{\sqrt{2}}-1\right)\left(\frac{1}{\sqrt{t+1}}-\frac{1}{\sqrt{t}}\right)\\
&\geq \varphi(n,d)+\frac{n-d+\sqrt{2}-2}{\sqrt{n-d}}-\frac{n-d+\sqrt{2}-1}{\sqrt{n-d+1}}+\frac{t+\sqrt{2}-1}{\sqrt{t+1}}-\frac{t+\sqrt{2}-2}{\sqrt{t}}\\
&\geq \varphi(n,d)+[f(n-d)-f(n-d+1)]-[f(t)-f(t+1)]\geq \varphi(n,d),
\end{aligned}$$

where $f(x)=\frac{x+\sqrt{2}-2}{\sqrt{x}}$ and the last inequality follows by Lemma 1(i) as $t\leq n-d$.

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

$$R(G')=\varphi(n-1,d),\ \ t=n-d,\ \ t-r=1\ \text{ and }\ d_1=d_2=2.$$

By the induction hypothesis, $G'\cong U^d_{n-1}$. Hence $G\cong U^d_n$.

Case 2. For every $u\in V_1\cap N_G(V_0')$, $|N(u)\setminus V_0|=1$.

In this case, $t\leq n-d-1$. Now we will show that $u\in\{v_2,v_d\}$. Otherwise, $u\notin V(P)\cup V(C)$. Let $G^+=G-uw_1-\cdots-uw_r+x_1w_1+\cdots+x_1w_r$. Then $G^+\in\mathscr{U}_{n,d}$ and $R(G^+)<R(G)$ by Lemma 3, a contradiction to the choice of G. Moreover, we may assume that $u=v_2$ and $w_1=v_1$ by Lemma 4. Hence $G-\{w_2,\ldots,w_r\}\cong P_{n-t+1,l}$, or $G-\{w_2,\ldots,w_r\}\cong Q_{n-t+1,i,j}$, or $G-\{w_2,\ldots,w_r\}\cong R_{n-t+1,i,l}$.

Subcase 2.1. $G-\{w_2,\ldots,w_r\}\cong P_{n-t+1,l}$.

In this subcase, if $l\geq 3$, then, by Lemma 1(ii), for $d=4$,

$$\begin{aligned}
R(G) &= \frac{n-5+\frac{1}{\sqrt{2}}}{\sqrt{n-4}}+\frac{1+\sqrt{6}}{2}\\
&= \varphi(n,4)+\frac{n-5+\frac{1}{\sqrt{2}}}{\sqrt{n-4}}-\frac{n-5+\sqrt{2}}{\sqrt{n-3}}+\frac{1+\sqrt{6}}{2}-\frac{1}{\sqrt{3}}-\frac{\sqrt{2}}{\sqrt{3}}\\
&\geq \varphi(n,4)+\frac{2+\frac{1}{\sqrt{2}}}{\sqrt{3}}-\frac{2+\sqrt{2}}{\sqrt{4}}+\frac{1+\sqrt{6}}{2}-\frac{1}{\sqrt{3}}-\frac{\sqrt{2}}{\sqrt{3}}>\varphi(n,4);
\end{aligned}$$

and for $d\geq 5$,

$$\begin{aligned}
R(G) &= \frac{t+\frac{1}{\sqrt{2}}}{\sqrt{t+1}}+\frac{3}{\sqrt{6}}+\frac{n-t-4}{2}\geq\frac{n-d-1+\frac{1}{\sqrt{2}}}{\sqrt{n-d}}+\frac{3}{\sqrt{6}}+\frac{d-3}{2}\\
&= \varphi(n,d)+\frac{n-d-1+\frac{1}{\sqrt{2}}}{\sqrt{n-d}}-\frac{n-d-1+\sqrt{2}}{\sqrt{n-d+1}}+1-\frac{1}{\sqrt{2}}\\
&\geq \varphi(n,d)+\frac{2+\frac{1}{\sqrt{2}}}{\sqrt{3}}-\frac{2+\sqrt{2}}{\sqrt{4}}+1-\frac{1}{\sqrt{2}}>\varphi(n,d).
\end{aligned}$$

If $l = 2$, then by an argument similar to the above, we have

$$R(G) = \begin{cases} \frac{t+\frac{1}{\sqrt{3}}}{\sqrt{t+1}} + \frac{2}{\sqrt{6}} + \frac{n-t-3}{2} \geq \frac{n-5+\sqrt{2}}{\sqrt{n-3}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}} = \varphi(n,4), & d = 4; \\ \frac{t+\frac{1}{\sqrt{3}}}{\sqrt{t+1}} + \frac{2}{\sqrt{6}} + \frac{n-t-3}{2} \geq \frac{n-d-1+\frac{1}{\sqrt{3}}}{\sqrt{n-d}} + \frac{2}{\sqrt{6}} + \frac{d-2}{2} > \varphi(n,d), & d \geq 5. \end{cases}$$

Subcase 2.2. $G - \{w_2, \ldots, w_r\} \cong Q_{n-t+1,i,j}$.

Subcase 2.2.1. $i + j = d$.

In this subcase, $i, j \geq 2$ by the assumption. Thus by Lemma 1(ii), for $i = 2$,

$$\begin{aligned} R(G) &= \frac{t+\frac{1}{\sqrt{4}}}{\sqrt{t+1}} + \frac{5}{\sqrt{8}} + \frac{n-t-5}{2} \geq \frac{n-d-1+\frac{1}{\sqrt{4}}}{\sqrt{n-d}} + \frac{5}{\sqrt{8}} + \frac{d-4}{2} \\ &= \varphi(n,d) + \frac{n-d-1+\frac{1}{\sqrt{4}}}{\sqrt{n-d}} - \frac{n-d-1+\sqrt{2}}{\sqrt{n-d+1}} + \begin{cases} \frac{5}{\sqrt{8}} - \frac{1+\sqrt{2}}{3}, & d = 4 \\ \frac{3\sqrt{2}+2-2\sqrt{6}}{4}, & d \geq 5 \end{cases} \\ &\geq \varphi(n,d) + \frac{2+\frac{1}{\sqrt{4}}}{\sqrt{3}} - \frac{2+\sqrt{2}}{\sqrt{4}} + \frac{3\sqrt{2}+2-2\sqrt{6}}{4} > \varphi(n,d); \end{aligned}$$

and for $i \geq 3$,

$$\begin{aligned} R(G) &= \frac{t+\frac{1}{\sqrt{2}}}{\sqrt{t+1}} + \frac{3}{\sqrt{2}} + \frac{n-t-6}{2} \geq \frac{n-d-1+\frac{1}{\sqrt{2}}}{\sqrt{n-d}} + \frac{3}{\sqrt{2}} + \frac{d-5}{2} \\ &= \varphi(n,d) + \frac{n-d-1+\frac{1}{\sqrt{2}}}{\sqrt{n-d}} - \frac{n-d-1+\sqrt{2}}{\sqrt{n-d+1}} + \sqrt{2} - \frac{\sqrt{6}}{2} \\ &\geq \varphi(n,d) + \frac{2+\frac{1}{\sqrt{2}}}{\sqrt{3}} - \frac{2+\sqrt{2}}{\sqrt{4}} + \sqrt{2} - \frac{\sqrt{6}}{2} > \varphi(n,d). \end{aligned}$$

Subcase 2.2.2. $i + j = d - 1$.

In this subcase, if $d = 4$, then $i = 2,\ j = 1$ and $t + 1 = n - 4$ or $n - 5$, thus for $t + 1 = n - 4$, we have

$$R(G) = \frac{n-5+\frac{1}{\sqrt{3}}}{\sqrt{n-4}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}} + \frac{1}{3} > \frac{n-5+\sqrt{2}}{\sqrt{n-3}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}} = \varphi(n,4).$$

and for $t + 1 = n - 5$, we have

$$R(G) = \frac{n-6+\frac{1}{\sqrt{3}}}{\sqrt{n-5}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}} + \frac{1}{3} + \frac{1}{2} > \frac{n-5+\sqrt{2}}{\sqrt{n-3}} + \frac{2}{\sqrt{6}} + \frac{1}{\sqrt{3}} = \varphi(n,4).$$

If $d \geq 5$, then by Lemma 1(ii), for $i \geq 3,\ j \geq 2$, we have

$$R(G) = \frac{t+\frac{1}{\sqrt{2}}}{\sqrt{t+1}} + \frac{4+\sqrt{3}}{\sqrt{6}} - \frac{19}{6} + \frac{n-t}{2} \geq \frac{n-d-1+\frac{1}{\sqrt{2}}}{\sqrt{n-d}} + \frac{4+\sqrt{3}}{\sqrt{6}} - \frac{8}{3} + \frac{d}{2}$$

$$
\begin{aligned}
&= \varphi(n,d) + \frac{n-d-1+\frac{1}{\sqrt{2}}}{\sqrt{n-d}} - \frac{n-d-1+\sqrt{2}}{\sqrt{n-d+1}} + \frac{\sqrt{6}-1}{6} \\
&\geq \varphi(n,d) + \frac{2+\frac{1}{\sqrt{2}}}{\sqrt{3}} - \frac{2+\sqrt{2}}{\sqrt{4}} + \frac{\sqrt{6}-1}{6} > \varphi(n,d);
\end{aligned}
$$

and for $i = 2,\ j \geq 2$,

$$
\begin{aligned}
R(G) &= \frac{t+\frac{1}{\sqrt{3}}}{\sqrt{t+1}} + \frac{1+\sqrt{3}}{\sqrt{2}} - \frac{8}{3} + \frac{n-t}{2} \geq \frac{n-d-1+\frac{1}{\sqrt{3}}}{\sqrt{n-d}} + \frac{1+\sqrt{3}}{\sqrt{2}} - \frac{13}{6} + \frac{d}{2} \\
&= \varphi(n,d) + \frac{n-d-1+\frac{1}{\sqrt{3}}}{\sqrt{n-d}} - \frac{n-d-1+\sqrt{2}}{\sqrt{n-d+1}} + \frac{1}{3} \\
&\geq \varphi(n,d) + \frac{2+\frac{1}{\sqrt{3}}}{\sqrt{3}} - \frac{2+\sqrt{2}}{\sqrt{4}} + \frac{1}{3} > \varphi(n,d);
\end{aligned}
$$

and for $i \geq 3,\ j = 1$,

$$
\begin{aligned}
R(G) &= \frac{t+\frac{1}{\sqrt{2}}}{\sqrt{t+1}} + \frac{3+\sqrt{2}}{\sqrt{6}} - \frac{8}{3} + \frac{n-t}{2} \geq \frac{n-d-1+\frac{1}{\sqrt{2}}}{\sqrt{n-d}} + \frac{3+\sqrt{2}}{\sqrt{6}} - \frac{13}{6} + \frac{d}{2} \\
&= \varphi(n,d) + \frac{n-d-1+\frac{1}{\sqrt{2}}}{\sqrt{n-d}} - \frac{n-d-1+\sqrt{2}}{\sqrt{n-d+1}} + \frac{1}{\sqrt{3}} + \frac{1}{3} - \frac{1}{\sqrt{2}} \\
&\geq \varphi(n,d) + \frac{2+\frac{1}{\sqrt{2}}}{\sqrt{3}} - \frac{2+\sqrt{2}}{\sqrt{4}} + \frac{1}{\sqrt{3}} + \frac{1}{3} - \frac{1}{\sqrt{2}} > \varphi(n,d).
\end{aligned}
$$

Subcase 2.2.3. $i + j \leq d - 2$.

In this subcase, $d \geq 5$. Thus by Lemma 1(ii), for $i \geq 3,\ j \geq 2$,

$$
\begin{aligned}
R(G) &= \frac{t+\frac{1}{\sqrt{2}}}{\sqrt{t+1}} + \frac{6+\sqrt{3}}{\sqrt{6}} + \frac{n-t-8}{2} \geq \frac{n-d-1+\frac{1}{\sqrt{2}}}{\sqrt{n-d}} + \frac{6+\sqrt{3}}{\sqrt{6}} + \frac{d-7}{2} \\
&= \varphi(n,d) + \frac{n-d-1+\frac{1}{\sqrt{2}}}{\sqrt{n-d}} - \frac{n-d-1+\sqrt{2}}{\sqrt{n-d+1}} + \frac{3}{\sqrt{6}} - \frac{2}{2} \\
&\geq \varphi(n,d) + \frac{2+\frac{1}{\sqrt{2}}}{\sqrt{3}} - \frac{2+\sqrt{2}}{\sqrt{4}} + \frac{3}{\sqrt{6}} - \frac{2}{2} > \varphi(n,d);
\end{aligned}
$$

and for $i = 2,\ j \geq 2$,

$$
\begin{aligned}
R(G) &= \frac{t+\frac{1}{\sqrt{3}}}{\sqrt{t+1}} + \frac{5+\sqrt{3}}{\sqrt{6}} + \frac{n-t-7}{2} \geq \frac{n-d-1+\frac{1}{\sqrt{3}}}{\sqrt{n-d}} + \frac{5+\sqrt{3}}{\sqrt{6}} + \frac{d-6}{2} \\
&= \varphi(n,d) + \frac{n-d-1+\frac{1}{\sqrt{3}}}{\sqrt{n-d}} - \frac{n-d-1+\sqrt{2}}{\sqrt{n-d+1}} + \frac{2}{\sqrt{6}} - \frac{1}{2} \\
&\geq \varphi(n,d) + \frac{2+\frac{1}{\sqrt{3}}}{\sqrt{3}} - \frac{2+\sqrt{2}}{\sqrt{4}} + \frac{2}{\sqrt{6}} - \frac{1}{2} > \varphi(n,d);
\end{aligned}
$$

and for $i \geq 3,\ j = 1$,

$$\begin{aligned} R(G) &= \frac{t+\frac{1}{\sqrt{2}}}{\sqrt{t+1}} + \frac{5+\sqrt{2}}{\sqrt{6}} + \frac{n-t-7}{2} \geq \frac{n-d-1+\frac{1}{\sqrt{2}}}{\sqrt{n-d}} + \frac{5+\sqrt{2}}{\sqrt{6}} + \frac{d-6}{2} \\ &= \varphi(n,d) + \frac{n-d-1+\frac{1}{\sqrt{2}}}{\sqrt{n-d}} - \frac{n-d-1+\sqrt{2}}{\sqrt{n-d+1}} + \frac{\sqrt{2}+1}{\sqrt{3}} - \frac{\sqrt{2}+1}{2} \\ &\geq \varphi(n,d) + \frac{2+\frac{1}{\sqrt{2}}}{\sqrt{3}} - \frac{2+\sqrt{2}}{\sqrt{4}} + \frac{\sqrt{2}+1}{\sqrt{3}} - \frac{\sqrt{2}+1}{2} > \varphi(n,d); \end{aligned}$$

and for $i = 2,\ j = 1$,

$$\begin{aligned} R(G) &= \frac{t+\frac{1}{\sqrt{3}}}{\sqrt{t+1}} + \frac{4+\sqrt{2}}{\sqrt{6}} + \frac{n-t-6}{2} \geq \frac{n-d-1+\frac{1}{\sqrt{3}}}{\sqrt{n-d}} + \frac{4+\sqrt{2}}{\sqrt{6}} + \frac{d-5}{2} \\ &= \varphi(n,d) + \frac{n-d-1+\frac{1}{\sqrt{3}}}{\sqrt{n-d}} - \frac{n-d-1+\sqrt{2}}{\sqrt{n-d+1}} + \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}} \\ &\geq \varphi(n,d) + \frac{2+\frac{1}{\sqrt{3}}}{\sqrt{3}} - \frac{2+\sqrt{2}}{\sqrt{4}} + \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}} > \varphi(n,d). \end{aligned}$$

Subcase 2.3. $G - \{w_2, \ldots, w_r\} \cong R_{n-t+1,i,l}$.

In this subcase, $d \geq 5$. Then by the similar calculations as above, we have

$$R(G) = \begin{cases} \frac{t+\frac{1}{\sqrt{2}}}{\sqrt{t+1}} + \frac{4}{\sqrt{6}} + \frac{1}{\sqrt{2}} + \frac{1}{3} + \frac{n-t-7}{2} > \varphi(n,d), & i \geq 3,\ l = 1; \\ \frac{t+\frac{1}{\sqrt{2}}}{\sqrt{t+1}} + \frac{6}{\sqrt{6}} + \frac{1}{\sqrt{2}} + \frac{n-t-8}{2} > \varphi(n,d), & i \geq 3,\ l \geq 2; \\ \frac{t+\frac{1}{\sqrt{3}}}{\sqrt{t+1}} + \frac{3}{\sqrt{6}} + \frac{1}{\sqrt{2}} + \frac{1}{3} + \frac{n-t-6}{2} > \varphi(n,d), & i = 2,\ l = 1; \\ \frac{t+\frac{1}{\sqrt{3}}}{\sqrt{t+1}} + \frac{5}{\sqrt{6}} + \frac{1}{\sqrt{2}} + \frac{n-t-7}{2} > \varphi(n,d), & i = 2,\ l \geq 2. \end{cases}$$

Therefore the proof of the theorem is complete. ■

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