Extremal trees for the Randić index

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Abstract. Graph theory has applications in various fields due to offering important tools such as topological indices. Among the topological indices, the Randić index is simple and of great importance. The Randić index of a graph $G$ can be expressed as $R(G) = \sum_{xy \in Y(G)} \frac{1}{\tau(x)\tau(y)}$, where $Y(G)$ represents the edge set and $\tau(x)$ is the degree of vertex $x$. In this paper, considering the importance of the Randić index and applications two-trees graphs, we determine the first two minimums among the two-trees graphs.

1 Introduction

Let $G$ be a simple graph having the vertex set $X = X(G)$ and the edge set $Y(G)$. Moreover, $\nu = |X(G)|$ and $m = |Y(G)|$. In this case, we say that $G$ is a graph of order $\nu$ and size $m$. The open neighborhood of vertex $x$ is defined as $\Omega_G(x) = \Omega(x) = \{y \in X(G) | xy \in Y(G)\}$ and the degree of $x$ is denoted by $|\Omega(x)| = \tau_G(x) = \tau(x)$. Suppose that $G$ is a graph with $x \in X(G)$ and $xy \in Y(G)$, then the graphs $G - x$ and $G - xy$ are obtained by removing the vertex $x$ and the edge $xy$ from $G$, respectively.

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The two-tree graph was first defined in the paper [9] in two steps as follows:

A. If \( s = 0 \) then \( \Theta_0 = K_2 \). In this case, we have a two-tree with two vertices.

B. Suppose \( \Theta_s \) is a two-tree produced during the \( s \)-th step. Then, graph \( \Theta_{s+1} \)

is generated during \((s+1)\)-step from graph \( \Theta_s \) by adding a new vertex adjacent to the two end vertices of an edge in \( \Theta_s \).

Some examples are shown in Figure 1. They will play an important role in the later development. Two-tree graphs have found many applications in complex networks see [6, 13] and more information see e.g. [5, 7, 8, 12].

![Figure 1: The graphs \( A_v \) and \( B_v \).](image)

In the past few decades, the topological indices due to their wide applications has been considered by many researchers. One of their oldest applications in chemistry was proposed by Wiener in the paper [11], which gave rise to the Wiener index. Due to the application of topological indices in various fields, many indices have been defined nowadays and their applications have been identified. Among those numerous indices [10], the Randić index was the most successful. The Randić index was first introduced in chemistry by Milan Randić in [4] to obtain the boiling point of paraffin and is defined as follows:

\[
R(G) = \sum_{xy \in Y(G)} \frac{1}{\sqrt{\tau(x)\tau(y)}}.
\]

As we mentioned before, due to the importance of the Randić index in other indices, it has been studied by many researchers over the years.

The Randić index has been considered extensively by researchers in the field of mathematics. For example, Lu et al. [3] discussed the Randić index quasi-tree graphs. Bermudo et al. [1] characterized Randić index tree with given domination number. In [2], the authors characterized Randić index for chemical trees. Motivated by the above line of research and the importance of the two-tree graphs, we in this paper intend to discuss the Randić index of two-
tree graphs. We establish the Randić index of two-tree graphs and determine the first two minimums among the two-tree graphs.

## 2 Some lemmas

In this section, we will prove a few lemmas that will help us achieve the main results.

**Lemma 1** Let $3 \leq g, h \leq \nu - 1$. For the function
\[
\varphi(g, h) = \frac{g - 1}{\sqrt{2g}} + \frac{h - 1}{\sqrt{2h}} - \frac{g - 2}{\sqrt{2(g - 1)}} - \frac{h - 2}{\sqrt{2(h - 1)}} + \frac{1}{\sqrt{gh}} - \frac{1}{\sqrt{(g - 1)(h - 1)}},
\]
we have $\varphi(g, h) \geq \varphi(\nu - 1, \nu - 1)$.

**Proof.** By deriving from function $\varphi(g, h)$, we have
\[
\frac{\partial \varphi(g, h)}{\partial g} = \frac{g - 2}{(2g - 2)^{3/2}} - \frac{g - 1}{(2g)^{3/2}}
- \frac{1}{\sqrt{2g - 2}} + \frac{1}{\sqrt{2g}} + \frac{h - 1}{2((g - 1)(h - 1))^{3/2}} - \frac{h}{2(gh)^{3/2}}
\]
and
\[
\frac{\partial}{\partial h} \frac{\partial \varphi(g, h)}{\partial g} = \frac{1}{2((g - 1)(h - 1))^{3/2}} - \frac{1}{2(gh)^{3/2}}
- \frac{3(g - 1)(h - 1)}{4((g - 1)(h - 1))^{5/2}} + \frac{3gh}{4(gh)^{5/2}}.
\]

Note that when $g, h \geq 3$, we get $\frac{\partial}{\partial g} \varphi(g, h) < 0$. Therefore, we have
\[
\frac{\partial \varphi(g, h)}{\partial g} \leq \frac{\partial \varphi(g, 3)}{\partial g}
= \frac{g - 2}{(2g - 2)^{3/2}} - \frac{g - 1}{(2g)^{3/2}}
- \frac{1}{\sqrt{2g - 2}} + \frac{1}{\sqrt{2g}} + \frac{1}{(2g - 2)^{3/2}} - \frac{3}{2(3g)^{3/2}}.
\]
It is not difficult to see that the above inequality is negative for $g \geq 3$. Hence, we derive $\frac{\partial \varphi(g, h)}{\partial g}, \frac{\partial \varphi(g, h)}{\partial h} < 0$ and that means $\varphi(g, h) \geq \varphi(\nu - 1, \nu - 1)$. \qed
Lemma 2 Let $3 \leq g, h \leq \nu - 2$. For the following function
\[
\psi(g, h) = \frac{1}{\sqrt{gh}} - \frac{1}{\sqrt{(g-1)(h-1)}} + \frac{1}{\sqrt{3g}} - \frac{1}{\sqrt{3(g-1)}} + \frac{1}{\sqrt{3h}} - \frac{1}{\sqrt{3(h-1)}} + \frac{g-3}{\sqrt{2g}} - \frac{g-3}{\sqrt{2(g-1)}} + \frac{h-3}{\sqrt{2h}} - \frac{h-3}{\sqrt{2(h-1)}},
\]
we have $\psi(g, h) \geq \psi(\nu - 2, \nu - 2)$.

Proof. By deriving from function $\psi(g, h)$, we have
\[
\frac{\partial \psi(g, h)}{\partial g} = \frac{g-3}{(2g-2)^{3/2}} - \frac{g-2}{(2g)^{3/2}} - \frac{1}{\sqrt{2g-2}} + \frac{1}{\sqrt{2g}} + \frac{h-1}{2((g-1)(h-1))^{3/2}} - \frac{h}{2(gh)^{3/2}} + \frac{3}{2(3g-3)^{3/2}} - \frac{3}{2(3g)^{3/2}}
\]
and
\[
\frac{\partial \partial \psi(g, h)}{\partial h \partial g} = \frac{1}{2((g-1)(h-1))^{3/2}} - \frac{1}{2(gh)^{3/2}} - \frac{3(g-1)(h-1)}{4((g-1)(h-1))^{5/2}} + \frac{3gh}{4(gh)^{5/2}}.
\]

Note that when $g, h \geq 3$, we get $\frac{\partial \psi(g, h)}{\partial g} < 0$. Hence, we have
\[
\frac{\partial \psi(g, h)}{\partial g} \leq \frac{\partial \psi(g, 3)}{\partial g} = \frac{g-3}{(2g-2)^{3/2}} - \frac{g-2}{(2g)^{3/2}} - \frac{1}{\sqrt{2g-2}} + \frac{1}{\sqrt{2g}} + \frac{3}{2(3g)^{3/2}} - \frac{3}{2(3g-3)^{3/2}}.
\]
It is not difficult to see that the above inequality is negative for $g \geq 3$. Hence, we obtain $\frac{\partial \psi(g, h)}{\partial g}, \frac{\partial \psi(g, h)}{\partial h} < 0$ and that means $\psi(g, h) \geq \psi(\nu - 1, \nu - 1)$. \qed

Lemma 3 For $\nu > 4$, we have
\[
h(\nu) = \frac{2(\nu - 4)}{\sqrt{2\nu - 4}} - \frac{(\nu - 5)}{\sqrt{2\nu - 6}} - \frac{v - 3}{\sqrt{2\nu - 2}} + \frac{2}{\sqrt{3\nu - 6}} - \frac{1}{\sqrt{3\nu - 9}} - \frac{1}{\sqrt{3\nu - 3}} + \frac{1}{\sqrt{\nu - 2}} - \frac{1}{\sqrt{\nu - 3}} + \frac{1}{\sqrt{(\nu - 3)(\nu - 2)}} - \frac{1}{\sqrt{(\nu - 2)(\nu - 1)}} > 0.
\]
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Proof. We know that

\[
\begin{align*}
    h(\nu) &= \frac{2(\nu - 4)}{\sqrt{2\nu - 4}} \frac{\nu - 5}{\sqrt{2\nu - 6}} - \frac{\nu - 3}{\sqrt{2\nu - 2}} + \frac{2}{\sqrt{3\nu - 6}} - \frac{1}{\sqrt{3\nu - 9}} \\
    & \quad - \frac{1}{\sqrt{3\nu - 3}} + \frac{1}{\nu - 2} - \frac{\nu - 3}{\sqrt{3(v - 3)(v - 2)}} - \frac{\nu - 2}{\sqrt{3(v - 2)(v - 1)}} \\
    &= \frac{2\sqrt{3\nu} - 8\sqrt{3} + 2\sqrt{2}}{\sqrt{6(v - 2)}} - \frac{\sqrt{3\nu} - 5\sqrt{3} + \sqrt{2}}{\sqrt{6(v - 3)}} - \frac{\sqrt{3\nu} - 3\sqrt{3} + \sqrt{2}}{\sqrt{6(v - 1)}} \\
    & \quad + \frac{1}{(\nu - 3)(\nu - 2)} \frac{1}{\sqrt{6(v - 2)(v - 1)}} > 0.
\end{align*}
\]

It is not difficult the above inequality holds for \( \nu \geq 4 \).

\[\square\]

3 Main results

In this section, we will discuss the Randić index of two-tree graphs and determine the first two minimums among this type of tree.

We start by proving a new result for Randić index.

Theorem 1 For a two-tree graph \( G \) with \( \nu \geq 4 \) vertices, we have

\[
R(G) \geq \frac{1}{\nu - 1} + \frac{2(\nu - 2)}{\sqrt{2(\nu - 1)}}.
\]

The equality holds if and only if \( G = A_\nu \) (see Figure 1).

Proof. We start the proof by inducing on \( \nu \). First, we assume that \( T_\nu \) is a two-tree of with four vertices. If \( G \) is a graph with four vertices, then this graph can be obtained from the complete graph with four vertices by removing an edge. By applying the definition of the Randić index for this graph, we get

\[
R(T_4) = 1.9663264951888 = \frac{2(\sqrt{6}+1)}{3}.
\]

We suppose our result holds for \( \nu - 1 \). Select a vertex of degree two from the graph \( T_\nu \), and we call it \( z \). It is not difficult to see that the graph \( T_\nu - z \) is a two-tree of \( \nu - 1 \) vertices.

By applying the induction hypothesis, we derive \( R(T_\nu - z) \geq R(A_{\nu - 1}) \) and the equality holds if and only if \( T_\nu - z = A_{\nu - 1} \). Hence, to complete the proof it suffices to show that \( R(T_\nu) \geq R(A_\nu) \).

Assume that \( x \) and \( y \) are two vertices adjacent to the vertex \( z \) in \( T_\nu \). Let \( \tau_{T_\nu}(x) = \emptyset, \tau_{T_\nu}(y) = \rho \) and \( \Omega_{T_\nu}(x) \setminus \{y, z\} = \{x_1, x_2, \ldots, x_{\rho - 2}\}, \Omega_{T_\nu}(y) \setminus \{x, z\} = \{y_1, y_2, \ldots, y_{\rho - 2}\} \). Then

\[
\begin{align*}
    R(T_\nu) &= \frac{1}{\nu - 1} + \frac{2(\nu - 2)}{\sqrt{2(\nu - 1)}} \frac{1}{\sqrt{(\nu - 3)(\nu - 2)}} + \frac{1}{\sqrt{(\nu - 2)(\nu - 1)}} > 0.
\end{align*}
\]
\{x_1, x_2, \ldots, x_{\rho-2}\}. Note that 3 ≤ ϑ, ρ ≤ υ - 1. By applying Lemma 1 and the induction hypothesis, we can write that

\[ R(T_\upsilon) = R(T_\upsilon - z) + \frac{1}{\sqrt{2\vartheta}} + \frac{1}{\sqrt{2\rho}} + \frac{1}{\sqrt{\vartheta\rho}} - \frac{1}{\sqrt{(\vartheta - 1)(\rho - 1)}} \]

\[ + \sum_{i=1}^{\vartheta-2} \left( \frac{1}{\sqrt{\vartheta\tau(x_i)}} - \frac{1}{\sqrt{(\vartheta - 1)\tau(x_i)}} \right) \]

\[ + \sum_{j=1}^{\rho-2} \left( \frac{1}{\sqrt{\rho\tau(y_j)}} - \frac{1}{\sqrt{(\rho - 1)\tau(y_j)}} \right) \]

\[ \geq R(A_{\upsilon-1}) + \frac{1}{\sqrt{2\vartheta}} + \frac{1}{\sqrt{2\rho}} + \frac{1}{\sqrt{\vartheta\rho}} - \frac{1}{\sqrt{(\vartheta - 1)(\rho - 1)}} \]

\[ + \sum_{i=1}^{\vartheta-2} \left( \frac{1}{\sqrt{2\vartheta}} - \frac{1}{\sqrt{2(\vartheta - 1)}} \right) + \sum_{j=1}^{\rho-2} \left( \frac{1}{\sqrt{2\rho}} - \frac{1}{\sqrt{2(\rho - 1)}} \right) \]

\[ = R(A_{\upsilon-1}) + \frac{\vartheta - 1}{\sqrt{2\vartheta}} + \frac{\rho - 1}{\sqrt{2\rho}} \]

\[ - \frac{\vartheta - 2}{\sqrt{2(\vartheta - 1)}} - \frac{\rho - 2}{\sqrt{2(\rho - 1)}} + \frac{1}{\sqrt{\vartheta\rho}} - \frac{1}{\sqrt{(\vartheta - 1)(\rho - 1)}} \]

\[ \geq R(A_{\upsilon-1}) + \frac{2(\upsilon - 2)}{\sqrt{2(\upsilon - 1)}} - \frac{2(\upsilon - 3)}{\sqrt{2(\upsilon - 2)}} + \frac{1}{\upsilon - 1} - \frac{1}{\sqrt{(\upsilon - 2)(\upsilon - 2)}} \]

\[ = \frac{1}{\upsilon - 2} + \frac{2(\upsilon - 3)}{\sqrt{2(\upsilon - 2)}} + \frac{2(\upsilon - 2)}{\sqrt{2(\upsilon - 1)}} - \frac{2(\upsilon - 3)}{\sqrt{2(\upsilon - 2)}} + \frac{1}{\upsilon - 1} - \frac{1}{\upsilon - 2} \]

\[ = R(A_\upsilon), \]

where the last equality is right if and only if \( T_\upsilon - z \cong A_{\upsilon-1}, \vartheta = \rho = \upsilon - 1 \) and \( d_{T_\upsilon}(x_i) = 2 \) for \( i = 1, 2, \ldots, \upsilon - 3 \) and that means \( T_\upsilon \cong A_\upsilon \). This completes the proof. \( \square \)

**Theorem 2** For a two-tree graph \( G \) with \( \upsilon \geq 5 \) vertices and \( G \not\cong A_\upsilon \), we have

\[ R(G) \geq \frac{1}{\sqrt{(\upsilon - 1)(\upsilon - 2)}} + \frac{\upsilon - 3}{\sqrt{2(\upsilon - 1)}} \]

\[ + \frac{\upsilon - 4}{\sqrt{2(\upsilon - 2)}} + \frac{1}{\sqrt{3(\upsilon - 1)}} + \frac{1}{\sqrt{3(\upsilon - 2)}} + \frac{\sqrt{6}}{6}. \]

The equality holds if and only if \( G \cong B_\upsilon \); see Figure 1.
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Proof. We begin the proof by inducing on \( v \). We assume that \( T_v \) is a two-tree with \( n \) vertices and \( T_v \not\cong A_v \). First, we assume that \( T_v \) is a two-tree of with five vertices. We obtain \( T_v \cong A_v \) or \( T_v \cong B_v \). Since \( T_v \not\cong A_v \), then \( G \cong B_v \).

Obviously \( R(T_5) = 2.4342869646372 = \sqrt{2} + \sqrt{3} + \sqrt{5} + \frac{1}{2} \). Suppose that theorem is true for \( v - 1 \). It is clear that a two-tree graph has at least two vertices of degree two. In addition, we have \( T_v \not\cong A_v \). Hence we choose a vertex of \( T_v \) with degree two, and call this vertex \( z \). We have \( T_v - z \cong A_{v-1} \). Clearly, the graph \( T_v - w \) is a two-tree with \( v - 1 \) vertices. By applying the induction hypothesis, we get that \( R(T_v - z) \geq R(B_{v-1}) \) and the equality holds if and only if \( T_v - z \cong B_{v-1} \). To complete the proof, it suffices for us to show that \( R(T_v) \geq R(B_v) \). Assume that \( x \) and \( y \) are two vertices adjacent to the vertex \( z \) in \( T_v \). Note that \( v \geq 5 \). Given that the graph is a two-tree graph, there should exist a vertex \( x \), adjacent to two vertices \( x \) and \( y \) satisfying \( \tau_{T_v} (x) \geq 3 \) (Otherwise, \( T_v - z \not\cong A_{v-1} \)). Let \( \tau_{T_v}(x) = \theta \), \( \tau_{T_v}(y) = \rho \), \( \tau_{T_v}(z) = \zeta \) and \( \Omega_{T_v}(x) \setminus \{x,z,\xi\} = \{x_1, x_2, \ldots, x_{\theta - 3}\} \), \( \Omega_{T_v}(y) \setminus \{x,z,\xi\} = \{y_1, y_2, \ldots, y_{\rho - 3}\} \). Note that \( 3 \leq \theta, \rho, \zeta \leq v - 1 \). For convenience here we assume that \( \theta \leq \rho \) and \( \max(\theta, \rho, \zeta) = \rho \). Since vertex \( \xi \) is not adjacent to the vertex \( z \), \( \zeta \leq \rho - 2 \) and \( \theta \leq \rho \leq v - 2 \). By applying Lemma 2, Lemma 3 and the induction hypothesis, we obtain

\[
R(T_v) = R(T_v - z) + \frac{1}{\sqrt{2\theta}} + \frac{1}{\sqrt{2\rho}} + \frac{1}{\sqrt{\theta \rho}} - \frac{1}{\sqrt{(\theta - 1)(\rho - 1)}} \\
+ \frac{1}{\sqrt{\theta \zeta}} - \frac{1}{\sqrt{(\theta - 1)\zeta}} + \frac{1}{\sqrt{\rho \zeta}} - \frac{1}{\sqrt{(\rho - 1)\zeta}} \\
+ \sum_{i=1}^{\theta - 3} \left( \frac{1}{\sqrt{\theta \tau(x_i)}} - \frac{1}{\sqrt{(\theta - 1)\tau(x_i)}} \right) \\
+ \sum_{j=1}^{\rho - 3} \left( \frac{1}{\sqrt{\rho \tau(y_j)}} - \frac{1}{\sqrt{(\rho - 1)\tau(y_j)}} \right) \\
\geq R(B_{v-1}) - \frac{1}{\sqrt{2\theta}} + \frac{1}{\sqrt{2\rho}} + \frac{1}{\sqrt{\theta \rho}} - \frac{1}{\sqrt{(\theta - 1)(\rho - 1)}} \\
+ \frac{1}{\sqrt{3\theta}} - \frac{1}{\sqrt{3(\theta - 1)}} + \frac{1}{\sqrt{3\rho}} - \frac{1}{\sqrt{3(\rho - 1)}} \\
+ \sum_{i=1}^{\theta - 3} \left( \frac{1}{\sqrt{2\theta}} - \frac{1}{\sqrt{2(\theta - 1)}} \right) + \sum_{j=1}^{\rho - 3} \left( \frac{1}{\sqrt{2\rho}} - \frac{1}{\sqrt{2(\rho - 1)}} \right)
\]
\[ R(B_{v-1}) + \frac{1}{\sqrt{3\delta}} - \frac{1}{\sqrt{(\delta - 1)(\rho - 1)}} \]
\[ \geq R(B_{v-1}) + \frac{1}{\sqrt{2\delta}} - \frac{1}{\sqrt{2(\delta - 1)}} + \frac{1}{\sqrt{2\rho}} - \frac{1}{\sqrt{2(\rho - 1)}} \]
\[ \geq R(B_{v-1}) + \frac{1}{\sqrt{2v - 4}} - \frac{2(v - 5)}{2v - 6} + \frac{1}{\sqrt{3v - 6}} - \frac{2}{\sqrt{3v - 9}} \]
\[ > R(B_\nu). \]

Hence, we derive \( \rho \leq v-1 \) and \( \max(\delta, \zeta) \leq v-2 \). Otherwise, we have \( T_\nu \not\cong A_\nu \).

Again by applying Lemma 2 and the induction hypothesis, we know that
\[ R(T_\nu) = R(T_\nu - z) + \frac{1}{\sqrt{2\delta}} + \frac{1}{\sqrt{2\rho}} - \frac{1}{\sqrt{(\delta - 1)(\rho - 1)}} \]
\[ + \sum_{i=1}^{\delta-3} \left( \frac{1}{\sqrt{\delta(\tau(x_i))}} - \frac{1}{\sqrt{(\delta - 1)(\tau(x_i))}} \right) \]
\[ + \sum_{j=1}^{\rho-3} \left( \frac{1}{\sqrt{\rho(\tau(y_j))}} - \frac{1}{\sqrt{(\rho - 1)(\tau(y_j))}} \right) \]
\[ > R(B_{v-1}) + \frac{1}{\sqrt{2\delta}} - \frac{1}{\sqrt{2(\delta - 1)}} + \frac{1}{\sqrt{2\rho}} - \frac{1}{\sqrt{2(\rho - 1)}} \]
\[ > R(B_\nu). \]
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\[ + \sum_{i=1}^{n-3} \left( \frac{1}{\sqrt{2\vartheta}} - \frac{1}{\sqrt{2(\vartheta-1)}} \right) + \sum_{j=1}^{n-3} \left( \frac{1}{\sqrt{2\rho}} - \frac{1}{\sqrt{2(\rho-1)}} \right) \]

\[ = R(B_{\nu-1}) + \frac{1}{\sqrt{3\vartheta}} - \frac{1}{\sqrt{3(\vartheta-1)}} + \frac{1}{\sqrt{3\rho}} - \frac{1}{\sqrt{3(\rho-1)}} \]

\[ = R(B_{\nu-1}) + \frac{1}{\sqrt{2(\vartheta-1)}} + \frac{\rho-2}{\sqrt{2\rho}} - \frac{\rho-3}{\sqrt{2(\rho-1)}} \]

\[ \geq R(B_{\nu-1}) + \frac{\nu-3}{\sqrt{2\nu-2}} - \frac{\nu-5}{\sqrt{2\nu-6}} + \frac{1}{\sqrt{3\nu-3}} - \frac{1}{\sqrt{3\nu-9}} \]

\[ = R(B_{\nu}). \]

It is easy to check that the last equality holds if and only if \( T_{\nu} = B_{\nu-1}, \vartheta = \nu - 2, \rho = \nu - 1, \zeta = 3 \) and \( \tau_{T_{\nu}}(x_i) = \tau_{T_{\nu}}(y_j) = 2 \) for \( i = 1, 2, \ldots, \nu - 3 \) and \( j = 1, 2, \ldots, \nu - 2 \), which means \( T_{\nu} \cong B_{\nu}. \)

\[ \square \]

4 Concluding Remark

In this article we have studied the Randić index for two-tree graphs and also discussed the first minimum and the second minimum of these graphs. However, discussions about the maximum of these graphs have not yet been resolved and seem to be difficult. In view of this, we make the following conjecture.

**Conjecture 1** If \( G \) is a two-tree graph with \( \nu \geq 6 \) vertices, then \( R(G) \leq \frac{\nu}{2} - k \) and the equality holds for graphs shown in Figure 2.
Figure 2: Graph described in conjecture 1 with $R(G) = \frac{\nu}{2} - k$ where, $k = 0.0716960995065$.

References


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