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The Maximum and Minimum Value of Exponential Randić Indices of Quasi-Tree Graph

Lei Qiu, Xijie Ruan, Yan Zhu*

School of Mathematics, East China University of Science and Technology, Shanghai, China
Email: 13122258370@163.com, *operationzy@163.com

Abstract

The exponential Randić index has important applications in the fields of biology and chemistry. The exponential Randić index of a graph G is defined as the sum of the weights $e^{\frac{1}{\sqrt{d(u)d(v)}}}$ of all edges uv of G, where $d(u)$ denotes the degree of a vertex u in G. The paper mainly provides the upper and lower bounds of the exponential Randić index in quasi-tree graphs, and characterizes the extremal graphs when the bounds are achieved.

Keywords

Exponential Randić Index, Quasi-Tree Graph, Extremal Value, Extremal Graphs

1. Introduction

Since the famous chemist Milan Randić proposed a structural descriptor called Randić index in 1975. The Randić index provides important references and guidance for the design and synthesis of new compounds, aiding chemists in better understanding the structure and properties of molecules, and thus facilitating the design and synthesis of molecular materials with specific properties and functions. Bollobás and Erdös [1] introduced the concept of the generalized Randić index and promoted the use of the indicator. For a simple connected graph $G = (V, E)$, V and E represent the set of vertices and edges of graph G, respectively. And $d(u)$ refers to the degree of a vertex u in G. The Randić index of the graph G is defined as

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}}.$$

There are a lot of researcher on the mathematical properties of the Randić index and general Randić index of a graph. Hu and Li [2] [3] studied the maximum and minimum values of the generalized Randić index in all trees containing n vertices. Wu and Zhang [4] provided the minimum value of the generalized Randić index at C_n in single-cycle graphs with n vertices when $\alpha > 0$. When $-1 \le \alpha < 0$, the minimum value is obtained at S_n^+. Pavlović [5] classified and discussed the maximum value of the zeroth-order Randić index in graphs without cycles, multiple edges, containing n vertices and m edges. Li and Zhao [6] provided the maximum, second maximum, third maximum, and minimum, second minimum, third minimum zeroth-order generalized Randić indices in trees, and characterized the corresponding extremal graphs. Zhang [7] provided the maximum, second maximum, third maximum, and minimum, second minimum, third minimum zeroth-order generalized Randić indices in single-cycle graphs, and characterized the corresponding extremal graphs. Jahanbani and Murat [8] studied the minimum value attained by this index in n-th order trees at the path.

The paper only considers simple connected graphs. Let $G - x$ represent the graph obtained by removing vertex x and its associated edges from graph G. If there exists a vertex $x \in V(G)$ such that the graph $G - x$ is a tree, then G is called a quasi-tree graph. This paper primarily focuses on the exponential Randić index of quasi-tree graphs, aiming to determine the maximum and minimum values of the exponential Randić index for quasi-tree graphs and provide corresponding extremal graphs. In practical applications, the exponential Randić index and the Wiener index can be analyzed from different perspectives to study the structure of graphs. The exponential Randić index can also play a role in the study of spectral properties, graph complexity, symmetry, centrality, reliability, and robustness of graphs. Deriving bounds of the exponential Randić index for quasi-tree graphs can aid in our understanding of chemical bonding, reaction mechanisms, and intermolecular interactions. The definition of exponential Randić index is as follows:

$$e^{\chi}(G) = \sum_{uv \in E(G)} e^{\frac{1}{\sqrt{d(u)d(v)}}}.$$

Lu and Guo [9] provided the upper and lower bounds of the Randić index for quasi-tree graphs:

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

They also provided the extremal graph as shown in **Figure 1**.

The equality holds if and only if $G \cong Q^0 T(n)$ and $G \cong Q^1 T(n)$.

Sun and Gao [10] studied the zeroth-order generalized Randić index of quasi-tree graphs and determined the extreme values of the zeroth-order general Randić index of quasi-trees with perfect matchings and p pendant vertices, and characterized the corresponding extremal graphs.
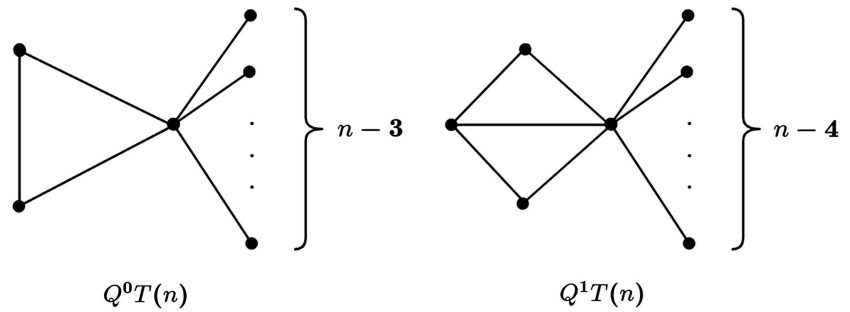
Figure 1. $Q^0 T(n)$ and $Q^1 T(n)$.

Based on the proofs in the paper, we can derive the following conclusion:

Conclusion 1. Let G be a quasi-tree graph with n vertices and $n \geq 3$. Then, there exists:

$$e^{\chi}(G) \leq 2e^{\frac{1}{\sqrt{2(n-1)}}} + (n+1)e^{\frac{1}{\sqrt{3(n-1)}}} + 2e^{\frac{1}{\sqrt{6}}} + (n-4)e^{\frac{1}{3}}.$$

The equality holds if and only if $G = U_n^0$ (**Figure 2**).

Conclusion 2. Let G be a quasi-tree graph with n vertices and $n \geq 3$. Then, there exists:

$$e^{\chi}(G) \geq (n-3)e^{\frac{1}{\sqrt{n-1}}} + 2e^{\frac{1}{\sqrt{2(n-1)}}} + e^{\frac{1}{2}}.$$

The equality holds if and only if $G \cong U_n^1$ (see **Figure 3**).

2. Preliminaries

In this section, we will delve into certain graph transformations that enhance the exponential Randić index. Additionally, we will present several lemmas. These transformations and lemmas will serve as valuable tools in substantiating our primary findings.

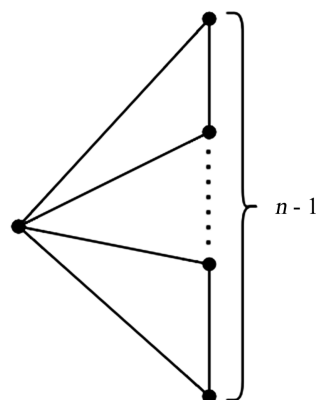**Lemma 2.1.** For integer $q \geq 0$, when $x \geq 2$, the function

$f(x) = e^{\frac{1}{\sqrt{(q+1)x}}} - e^{\frac{1}{\sqrt{qx}}}$ is monotonically increasing.

Proof. For $x \geq 2$, it can be obtained that:

$$\frac{\mathrm{d}f(x)}{\mathrm{d}x} = \frac{qe^{\frac{1}{\sqrt{qx}}}}{2(xq)^{\frac{3}{2}}} - \frac{(q+1)e^{\frac{1}{\sqrt{(q+1)x}}}}{2((q+1)x)^{\frac{3}{2}}}$$

$$= \frac{1}{2x^{\frac{3}{2}}} \left(\frac{qe^{\frac{1}{\sqrt{qx}}}}{q^{\frac{3}{2}}} - \frac{(q+1)e^{\frac{1}{\sqrt{(q+1)x}}}}{(q+1)^{\frac{3}{2}}} \right)$$

$$= \frac{1}{2x^{\frac{3}{2}}} \left(\frac{e^{\frac{1}{\sqrt{qx}}}}{\sqrt{q}} - \frac{e^{\frac{1}{\sqrt{(q+1)x}}}}{\sqrt{q+1}} \right) > 0$$

First, we introduce some special graph transformations.
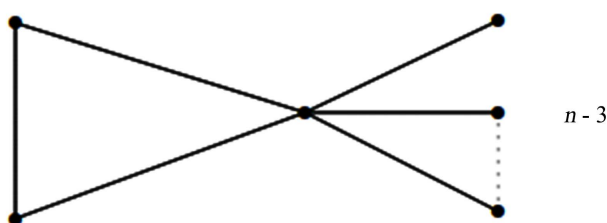
$$U_n^0$$

Figure 2. U_n^0.

Figure 3. U_n^1.

Graph transformation 1: In graph G_1, select a subgraph H_1 and add a new vertex v_1 and v_2 to a vertex u in it, such that v_1 and v_2 are adjacent to u, and their degrees are 2, 3, or 4, respectively. Then, attach two paths to G_1 to obtain a new graph $K_1 = G_1 - uw_1 + u_a w_1$. The resulting new graph K_1 is called the graph obtained from G_1 through graph transformation 1 (as shown in **Figure 4**).

Lemma 2.2. If K_1 is obtained from G_1 through graph transformation 1, then $e^\chi(G_1) < e^\chi(K_1)$.

Proof. Through graph transformation 1, let $d(v_1) = d_1$, $d(v_2) = d_2$, we can obtain:

$$
\begin{aligned}
e^\chi(K_1) - e^\chi(G_1) &= e^{\frac{1}{\sqrt{3d_1}}} + e^{\frac{1}{\sqrt{3d_2}}} + e^{\frac{1}{\sqrt{6}}} + (a+b-2)e^{\frac{1}{2}} + e^{\frac{1}{\sqrt{2}}} \\
&\quad - e^{\frac{1}{\sqrt{4d_1}}} - e^{\frac{1}{\sqrt{4d_2}}} - 2e^{\frac{1}{\sqrt{8}}} - (a+b-4)e^{\frac{1}{2}} - 2e^{\frac{1}{\sqrt{2}}} \\
&= e^{\frac{1}{\sqrt{3d_1}}} - e^{\frac{1}{\sqrt{4d_1}}} + e^{\frac{1}{\sqrt{3d_2}}} - e^{\frac{1}{\sqrt{4d_2}}} + e^{\frac{1}{\sqrt{6}}} - 2e^{\frac{1}{\sqrt{8}}} + 2e^{\frac{1}{2}} - e^{\frac{1}{\sqrt{2}}} \\
&> 0.0625 > 0
\end{aligned}
$$

When $x \geq 2$, the function $f(x) = e^{\frac{1}{\sqrt{(q+1)x}}} - e^{\frac{1}{\sqrt{qx}}}$ is monotonically increasing. Therefore:

$$e^\chi(K_1) - e^\chi(G_1) > 0.0265,$$
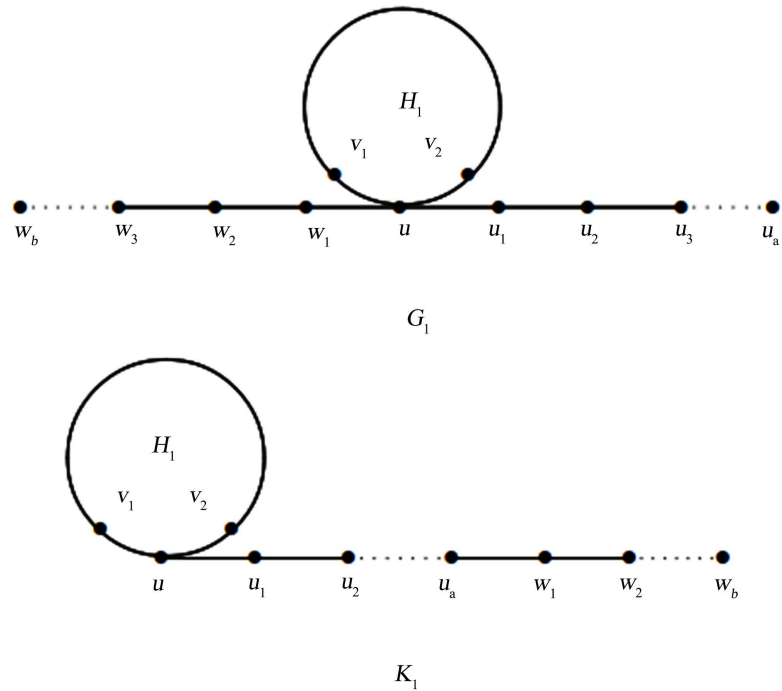
The lemma holds.

Figure 4. Graph transformation 1.

Graph transformation 2: Given a path $P = v_1v_2\cdots v_{t-1}v_t$ connected to the vertex v_1, then in the graph G_2, select two adjacent vertices u and w different from v_2, such that $d(u)=2$ or $d(u)=3$, $d(w)=2$ or $d(w)=3$, and $d(u) \neq d(w)$. Finally, by removing some edges from graph G_2 and adding some new edges, a new graph K_2 is formed. We refer to this process as graph transformation 2 (**Figure 5**).

Lemma 2.3. If K_2 is obtained from G_2 through graph transformation 2, then $e^{\chi}(G_2) < e^{\chi}(K_2)$.

Proof. Through graph transformation 2, let $d(u)=d_1$, $d(w)=d_2$, and $d(u) \neq d(w)$, we can obtain:

$$e^{\chi}(K_2) - e^{\chi}(G_2)$$

$$= e^{\frac{1}{\sqrt{2d_1}}} + e^{\frac{1}{\sqrt{2d_2}}} + (t-1)e^{\frac{1}{2}} - e^{\frac{1}{\sqrt{3d_1}}} - e^{\frac{1}{\sqrt{3d_2}}} - e^{\frac{1}{\sqrt{6}}} - e^{\frac{1}{\sqrt{2}}} - (t-3)e^{\frac{1}{2}}$$

$$= e^{\frac{1}{\sqrt{2d_1}}} - e^{\frac{1}{\sqrt{3d_1}}} + e^{\frac{1}{\sqrt{2d_2}}} - e^{\frac{1}{\sqrt{3d_2}}} + 2e^{\frac{1}{2}} - e^{\frac{1}{\sqrt{6}}} - e^{\frac{1}{\sqrt{2}}}$$

$$> 0.0183 > 0$$

The lemma holds.

Graph transformation 3: For a given graph G_3 and three paths P_1, P_2, and P_3, if the endpoints connected by path P_1 are u and a, the endpoints connected by path P_2 are v and b, and the endpoints connected by path P_3 are w and c, and it satisfies $d(u)=d_1$ (where d_1 equals 2 or 3) and $d(v)=d_2$ (where d_2 equals 2 or 3), then by connecting and disconnecting edges in a certain manner, a new graph K_3 can be obtained from the graph. This operation can be referred to as graph transformation 3 (as shown in **Figure 6**).
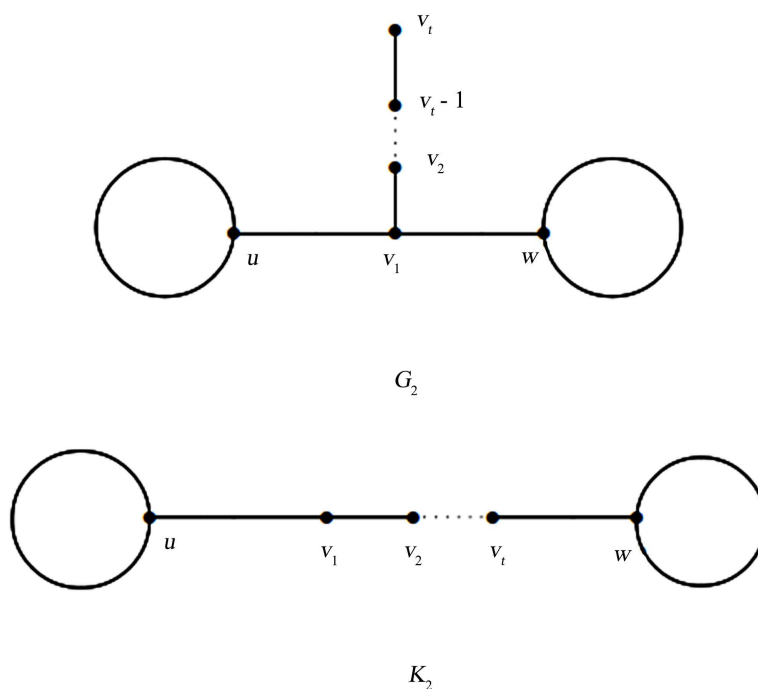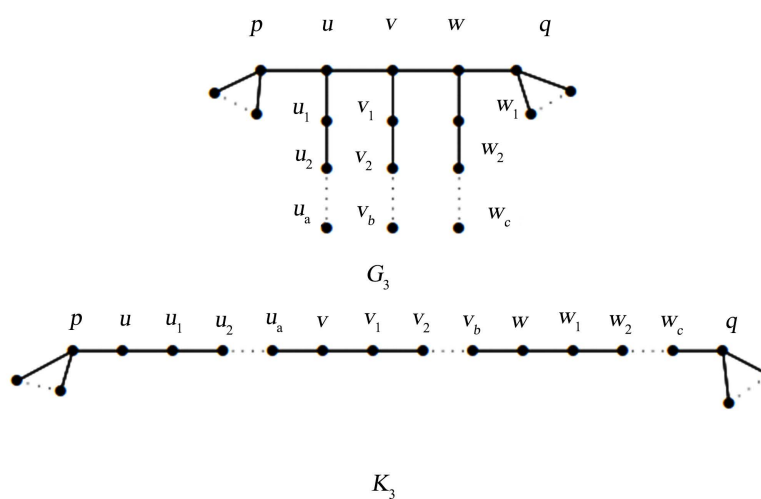
Figure 5. Graph transformation 2.

Figure 6. Graph transformation 3.

Lemma 2.4. If K_3 is obtained from G_3 through graph transformation 3, then $e^\chi(G_3) < e^\chi(K_3)$.

Proof. Let $d(p) = d_1$, $d(q) = d_2$, we can obtain:

$$e^\chi(K_3) - e^\chi(G_3) = e^{\frac{1}{\sqrt{2d_1}}} + (a+b+c+2)e^{\frac{1}{2}} + e^{\frac{1}{\sqrt{2d_2}}} - e^{\frac{1}{\sqrt{3d_1}}}$$

$$- e^{\frac{1}{\sqrt{3d_2}}} - 2e^{\frac{1}{3}} - 3e^{\frac{1}{\sqrt{6}}} - 3e^{\frac{1}{\sqrt{2}}} - (a+b+c-6)e^{\frac{1}{2}}$$

$$= e^{\frac{1}{\sqrt{2d_1}}} - e^{\frac{1}{\sqrt{3d_1}}} + e^{\frac{1}{\sqrt{2d_2}}} - e^{\frac{1}{\sqrt{3d_2}}} + 8e^{\frac{1}{2}} - 2e^{\frac{1}{3}} - 3e^{\frac{1}{\sqrt{6}}} - 3e^{\frac{1}{\sqrt{2}}}$$

$$> 0.0188 > 0$$

The lemma holds.

To further study the exponential Randić index in quasi-tree graphs, here we first present quasi-tree graphs for $n = 4$ and $n = 5$, and then calculate the exponential Randić index for each quasi-tree graph, observing the patterns.

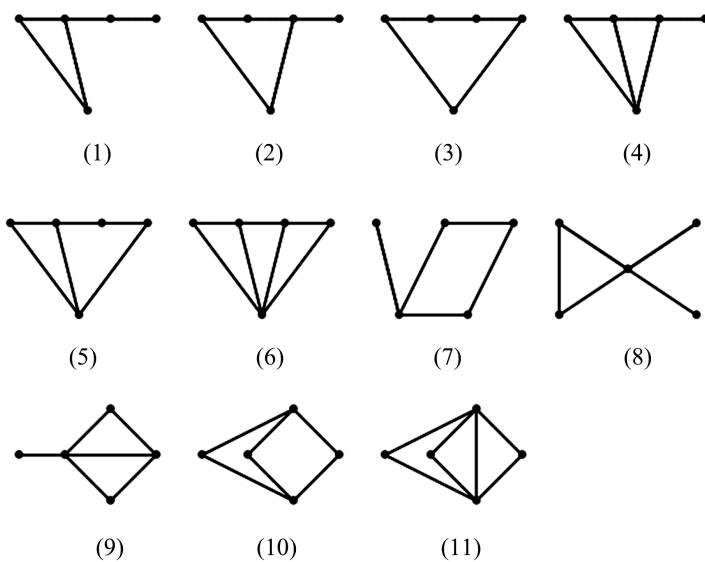When $n = 4$, quasi-tree graphs with cycles are shown in **Figure 7**.

When $n = 4$, the maximum value of the exponential Randić index for quasi-tree graphs is $4e^{\frac{1}{\sqrt{6}}} + e^{\frac{1}{3}} = 7.4123$, and the corresponding extremal graph is shown in **Figure 7(3)**. When $n = 4$, the minimum value of the exponential Randić index for quasi-tree graphs with cycles is $2e^{\frac{1}{\sqrt{6}}} + e^{\frac{1}{\sqrt{3}}} + e^{\frac{1}{2}} = 6.4384$, and the corresponding extremal graph is shown in **Figure 7(1)**, and the exponential Randić index for **Figure 7(2)** is $4e^{\frac{1}{2}} = 6.5949$.

When $n = 5$, quasi-tree graphs with cycles are shown in **Figure 8**.

The exponential Randić index for (1) is $3e^{\frac{1}{\sqrt{6}}} + e^{\frac{1}{2}} + e^{\frac{1}{\sqrt{2}}} = 8.1893$; the exponential Randić index for (2) is $2e^{\frac{1}{\sqrt{6}}} + 2e^{\frac{1}{2}} + e^{\frac{1}{\sqrt{3}}} = 8.0871$; the exponential Randić index for (3) is $5e^{\frac{1}{2}} = 8.2436$; the exponential Randić index for (4) is $2e^{\frac{1}{\sqrt{6}}} + 3e^{\frac{1}{3}} + e^{\frac{1}{\sqrt{3}}} = 8.976$; the exponential Randić index for (5) is $4e^{\frac{1}{\sqrt{6}}} + e^{\frac{1}{3}} + e^{\frac{1}{2}} = 9.0611$; the exponential Randić index for (6) is $2e^{\frac{1}{\sqrt{8}}} + 2e^{\frac{1}{\sqrt{12}}} + 2e^{\frac{1}{\sqrt{6}}} + e^{\frac{1}{3}} = 9.9215$; the exponential Randić index for (7) is $2e^{\frac{1}{\sqrt{6}}} + e^{\frac{1}{\sqrt{3}}} + 2e^{\frac{1}{2}} = 8.0871$; the exponential Randić index for (8) is $2e^{\frac{1}{\sqrt{8}}} + 3e^{\frac{1}{2}} = 7.7944$; the exponential Randić index for (9) is $2e^{\frac{1}{\sqrt{6}}} + e^{\frac{1}{\sqrt{12}}} + 2e^{\frac{1}{\sqrt{8}}} + e^{\frac{1}{2}} = 8.8400$; the exponential Randić index for (10) is $6e^{\frac{1}{\sqrt{6}}} = 9.0251$; the exponential Randić index for (11) is $6e^{\frac{1}{\sqrt{8}}} + e^{\frac{1}{4}} = 9.8287$.

(1)   (2)   (3)
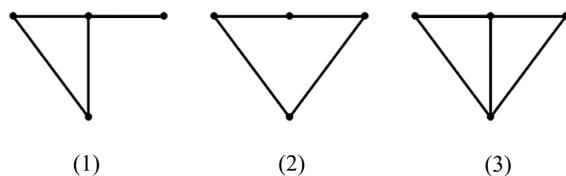
Figure 7. Quasi-tree graphs with cycles for $n = 4$.

(1)   (2)   (3)   (4)

(5)   (6)   (7)   (8)

(9)   (10)   (11)

Figure 8. Quasi-tree graphs with cycles for $n = 5$.

When $n = 5$, the maximum value of the exponential Randić index for quasi-tree graphs is $2e^{\frac{1}{\sqrt{8}}} + 2e^{\frac{1}{\sqrt{12}}} + 2e^{\frac{1}{\sqrt{6}}} + e^{\frac{1}{3}} = 9.9215$, and the corresponding extremal graph is shown in **Figure 8(6)**. When $n = 5$, the minimum value of the exponential Randić index for quasi-tree graphs is $2e^{\frac{1}{\sqrt{8}}} + 3e^{\frac{1}{2}} = 7.7944$, and the corresponding extremal graph is shown in **Figure 8(8)**. It is not difficult to see that when $n = 5$, quasi-tree graphs with cycles can be clearly divided into three categories based on the number of edges, among which:

Number of edges is 5: (1) (2) (3) (7) (8),

Number of edges is 6: (4) (5) (9) (10),

Number of edges is 7: (6) (11).

Lemma 2.5. Monotonic properties of three functions:

1) The function $g_1(x) = e^{\frac{1}{\sqrt{x}}}$ is monotonically decreasing for $x \geq 2$.

2) The function $g_2(x) = e^{\frac{1}{\sqrt{2}}} - e^{\frac{1}{\sqrt{x-1}}}$ is monotonically increasing for $x \geq 2$.

3) The function $g_3(x) = \left(1 - \frac{1}{2} x^{-\frac{1}{2}}\right) e^{\frac{1}{\sqrt{x}}}$ is monotonically decreasing for $x \geq 2$.

Proof.

1) By definition of $g(t) = e^t$, $t(x) = \left(\sqrt{x}\right)^{-1}$ it can be derived that is monotonically decreasing for $x \geq 2$.

2) Based on the conclusion of (1) and the expression of the function $g_2(x)$, it can be concluded that $g_2(x)$ is monotonically increasing for $x \geq 2$.

3) For $x \geq 2$, through a series of transformations, it can be proved that $g_3(x)$ is monotonically decreasing for $x \geq 2$.

$$
\begin{aligned}
\frac{dg_3(x)}{dx} &= \frac{1}{4} x^{-\frac{3}{2}} e^{\frac{1}{\sqrt{x}}} - \frac{1}{2} x^{-\frac{3}{2}} \left(1 - \frac{1}{2} x^{-\frac{1}{2}}\right) e^{\frac{1}{\sqrt{x}}} \\
&= \frac{1}{4} x^{-\frac{3}{2}} e^{\frac{1}{\sqrt{x}}} - \left(\frac{1}{2} - \frac{1}{4} x^{-\frac{1}{2}}\right) x^{-\frac{3}{2}} e^{\frac{1}{\sqrt{x}}} \\
&= e^{\frac{1}{\sqrt{x}}} x^{-\frac{3}{2}} \left(\frac{1}{4} - \frac{1}{2} + \frac{1}{4} x^{-\frac{1}{2}}\right) \\
&= \frac{1}{4} e^{\frac{1}{\sqrt{x}}} x^{-\frac{3}{2}} \left(\frac{1}{\sqrt{x}} - 1\right) \\
&< 0
\end{aligned}
$$

Therefore, (3) holds true.

Lemma 2.6. When $x \geq 2$, the function $f(x) = \frac{1}{2} e^{\frac{1}{\sqrt{x}}} - \frac{\sqrt{2}}{4} e^{\frac{1}{\sqrt{2x}}}$ is monotonically decreasing.

Proof. When $x \geq 2$, it can be derived that:

$$
\begin{aligned}
\frac{df(x)}{dx} &= -\frac{1}{4} e^{\frac{1}{\sqrt{x}}} x^{-\frac{3}{2}} + \frac{\sqrt{2}}{4} (2x)^{-\frac{3}{2}} e^{\frac{1}{\sqrt{2x}}} \\
&= \frac{1}{8} x^{-\frac{3}{2}} e^{\frac{1}{\sqrt{2x}}} - \frac{1}{4} x^{-\frac{3}{2}} e^{\frac{1}{\sqrt{x}}} \\
&< 0
\end{aligned}
$$

Hence, the function $f(x)$ is monotonically decreasing.

Lemma 2.7. Let x and y be positive integers, $x \geq 1$, $y \geq 2$, then:

$$l(x,y) = e^{\frac{1}{\sqrt{y}}} + x\left(e^{\frac{1}{\sqrt{y}}} - e^{\frac{1}{\sqrt{y-1}}}\right) + (y-1-x)\left(e^{\frac{1}{\sqrt{2y}}} - e^{\frac{1}{\sqrt{2(y-1)}}}\right)$$

is monotonically decreasing with respect to *x*.

Proof. For $x \geq 1$ and $y \geq 2$, it can be derived that

$$\frac{\partial l(x,y)}{\partial x} = \left(e^{\frac{1}{\sqrt{y}}} - e^{\frac{1}{\sqrt{y-1}}}\right) - \left(e^{\frac{1}{\sqrt{2y}}} - e^{\frac{1}{\sqrt{2(y-1)}}}\right)$$

By Lemma 2.1, $\dfrac{\partial l(x,y)}{\partial x}$, $l(x,y)$ is monotonically decreasing with respect to *x*.

Lemma 2.8. For $x \geq 2$ the function

$$f(x) = e^{\frac{1}{\sqrt{x}}} + (x-2)\left(e^{\frac{1}{\sqrt{x}}} - e^{\frac{1}{\sqrt{x-1}}}\right) + \left(e^{\frac{1}{\sqrt{2x}}} - e^{\frac{1}{\sqrt{2(x-1)}}}\right)$$

is monotonically decreasing with respect to *x*.

Proof. For $x \geq 2$, by applying Lemma 2.3.1 (3) and Lemma 2.2.1, it can be derived that

$$\frac{\mathrm{d}f(x)}{\mathrm{d}x} = e^{\frac{1}{\sqrt{x}}}\left(-\frac{1}{2}x^{-\frac{3}{2}}\right) + \left(e^{\frac{1}{\sqrt{x}}} - e^{\frac{1}{\sqrt{x-1}}}\right) + (x-2)\left[e^{\frac{1}{\sqrt{x}}}\left(-\frac{1}{2}x^{-\frac{3}{2}}\right)\right.$$

$$\left. - e^{\frac{1}{\sqrt{x-1}}}\left(-\frac{1}{2}(x-1)^{-\frac{3}{2}}\right)\right] - e^{\frac{1}{\sqrt{2x}}}(2x)^{-\frac{3}{2}} + e^{\frac{1}{\sqrt{2(x-1)}}}[2(x-1)]^{-\frac{3}{2}}$$

$$= -\frac{1}{2}e^{\frac{1}{\sqrt{x}}}x^{-\frac{3}{2}} + \left(e^{\frac{1}{\sqrt{x}}} - e^{\frac{1}{\sqrt{x-1}}}\right) + (x-2)\left[-\frac{1}{2}e^{\frac{1}{\sqrt{x}}}x^{-\frac{3}{2}} + \frac{1}{2}e^{\frac{1}{\sqrt{x-1}}}(x-1)^{-\frac{3}{2}}\right]$$

$$- \frac{\sqrt{2}}{4}e^{\frac{1}{\sqrt{2x}}}x^{-\frac{3}{2}} + \frac{\sqrt{2}}{4}e^{\frac{1}{\sqrt{2(x-1)}}}(x-1)^{-\frac{3}{2}}$$

$$= \left(\frac{1}{2}e^{\frac{1}{\sqrt{x}}} - \frac{\sqrt{2}}{4}e^{\frac{1}{\sqrt{2x}}}\right)x^{-\frac{3}{2}} + \left(\frac{\sqrt{2}}{4}e^{\frac{1}{\sqrt{2(x-1)}}} - e^{\frac{1}{\sqrt{x-1}}}\right)(x-1)^{-\frac{3}{2}} + e^{\frac{1}{\sqrt{x}}}$$

$$- e^{\frac{1}{\sqrt{x-1}}} - \frac{1}{2}e^{\frac{1}{\sqrt{x}}}x^{-\frac{3}{2}} + \frac{1}{2}e^{\frac{1}{\sqrt{x-1}}}x(x-1)^{-\frac{3}{2}}$$

$$\leq \left(\frac{1}{2}e^{\frac{1}{\sqrt{x}}} - \frac{\sqrt{2}}{4}e^{\frac{1}{\sqrt{2x}}}\right)(x-1)^{-\frac{3}{2}} + \left(\frac{\sqrt{2}}{4}e^{\frac{1}{\sqrt{2(x-1)}}} - e^{\frac{1}{\sqrt{x-1}}}\right)(x-1)^{-\frac{3}{2}}$$

$$+ e^{\frac{1}{\sqrt{x}}} - e^{\frac{1}{\sqrt{x-1}}} - \frac{1}{2}e^{\frac{1}{\sqrt{x}}}x^{-\frac{3}{2}} + \frac{1}{2}e^{\frac{1}{\sqrt{x-1}}}x(x-1)^{-\frac{3}{2}}$$

$$= \left(e^{\frac{1}{\sqrt{x}}} - \frac{\sqrt{2}}{4}e^{\frac{1}{\sqrt{2x}}}\right)(x-1)^{-\frac{3}{2}} + \left(\frac{\sqrt{2}}{4}e^{\frac{1}{\sqrt{2(x-1)}}} - e^{\frac{1}{\sqrt{x-1}}}\right)(x-1)^{-\frac{3}{2}} + e^{\frac{1}{\sqrt{x}}}$$

$$- e^{\frac{1}{\sqrt{x-1}}} - \frac{1}{2}e^{\frac{1}{\sqrt{x}}}x^{-\frac{3}{2}} + \frac{1}{2}e^{\frac{1}{\sqrt{x-1}}}x(x-1)^{-\frac{3}{2}} - \frac{1}{2}e^{\frac{1}{\sqrt{x}}}(x-1)^{-\frac{3}{2}}$$

$$= \left(\frac{1}{2} e^{\frac{1}{\sqrt{x}}} - \frac{\sqrt{2}}{4} e^{\frac{1}{\sqrt{2x}}} + \frac{\sqrt{2}}{4} e^{\frac{1}{\sqrt{2(x-1)}}} - \frac{1}{2} e^{\frac{1}{\sqrt{x-1}}} \right) (x-1)^{-\frac{3}{2}} + e^{\frac{1}{\sqrt{x}}} - e^{\frac{1}{\sqrt{x-1}}}$$

$$- \frac{1}{2 e^{\frac{1}{\sqrt{x}}} x^{-\frac{1}{2}}} - \frac{1}{2} e^{\frac{1}{\sqrt{x}}} (x-1)^{-\frac{3}{2}} + \frac{1}{2} e^{\frac{1}{\sqrt{x-1}}} x (x-1)^{-\frac{3}{2}} + \frac{1}{2} \left(e^{\frac{1}{\sqrt{x}}} - e^{\frac{1}{\sqrt{x-1}}} \right)(x-1)^{-\frac{3}{2}}$$

$$\leq e^{\frac{1}{\sqrt{x}}} - e^{\frac{1}{\sqrt{x-1}}} - \frac{1}{2} e^{\frac{1}{\sqrt{x}}} x^{-\frac{1}{2}} - \frac{1}{2} e^{\frac{1}{\sqrt{x}}} (x-1)^{-\frac{3}{2}} + \frac{1}{2} e^{\frac{1}{\sqrt{x-1}}} x (x-1)^{-\frac{3}{2}}$$

$$+ \frac{1}{2} \left(e^{\frac{1}{\sqrt{x}}} - e^{\frac{1}{\sqrt{x-1}}} \right)(x-1)^{-\frac{3}{2}}$$

$$< 0$$

Hence, $f(x)$ is monotonically decreasing.

Lemma 2.9. Let *n* be a positive integer and $n \geq 6$, it can be obtained

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

Proof. Let

$$f(n) = 3 e^{\frac{1}{\sqrt{2(n-2)}}} - e^{\frac{1}{\sqrt{2(n-3)}}} - e^{\frac{1}{\sqrt{2(n-1)}}} - (n-3)\left(e^{\frac{1}{\sqrt{n-1}}} - e^{\frac{1}{\sqrt{n-2}}} \right) - (n-4)\left(e^{\frac{1}{\sqrt{n-3}}} - e^{\frac{1}{\sqrt{n-2}}} \right).$$

We use MATLAB to calculate and plot the function graph to determine the validity of the inequality.

Define the horizontal axis variable as a one-dimensional array *x*, with the first element being 3, an increment of 0.01, and the final element being 15 (as shown in **Figure 9**).
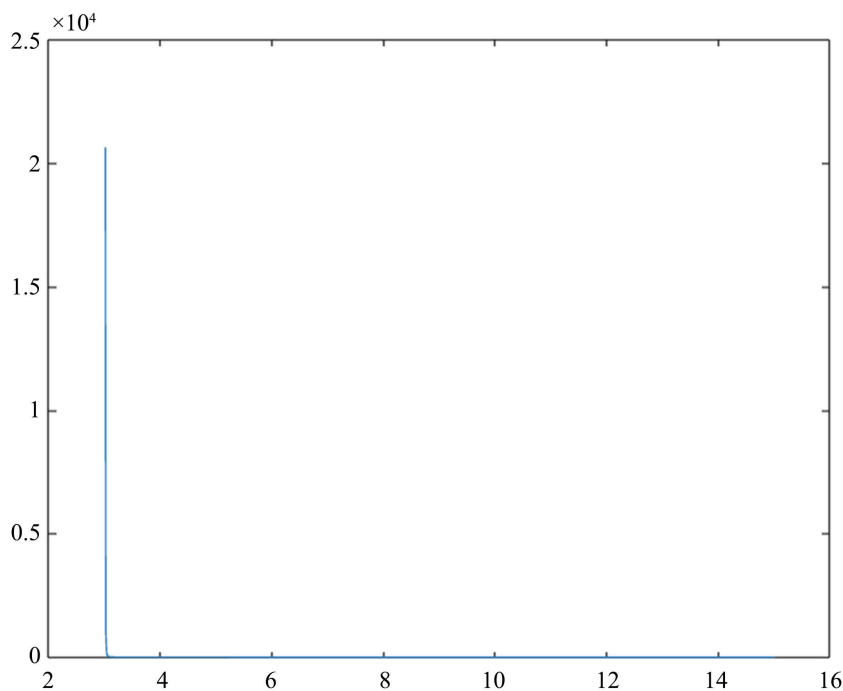
Figure 9. The graph of the function.

From the figure, it can be seen that the graph of $f(n)$ always lies above the coordinate axis. Calculated by MATLAB, the point of intersection of $f(n)$ and the horizontal axis is (0, −27852563104487148.539894396758705−23751291381668762.757332046522084 * i). Therefore, when $n \geq 6$, $f(n) \geq 0$ always holds true.

3. Main Results

In this section, we will give the upper and lower bounds on the exponential Randić indices of quasi-tree graph.

3.1. The Upper Bounds and Extreme Graph

Theorem 3.1. If T is a tree graph with n vertices, then T is not the maximum value of e^{χ} in T_n.

Proof. P_n can be continuously transformed from T through graph transformation 1, graph transformation 2, and graph transformation 3, and by Lemma 2.2, Lemma 2.3, and Lemma 2.4. Therefore, $G(T) < G(P_n)$.

The theorem is proven.

Theorem 3.2. Let G be a quasi-tree graph with n vertices, then:

$$e^{\chi}(G) \leq 2e^{\frac{1}{\sqrt{2(n-1)}}} + (n+1)e^{\frac{1}{\sqrt{3(n-1)}}} + 2e^{\frac{1}{\sqrt{6}}} + (n-4)e^{\frac{1}{3}}.$$

Proof. When the number of edges is equal to $n-1$, G is a tree graph. By Theorem 3.1, it is known that in an n-order tree graph, e^{χ} attains its maximum value on the path P_n. At this point:

$$e^{\chi}(G) \leq (n-3)e^{\frac{1}{2}} + 2e^{\frac{1}{\sqrt{2}}}.$$

When G is a cycle graph, increasing the pendant edges will decrease the value of the exponential Randić index. By repeatedly applying Lemma 2.2, Lemma 2.3, and Lemma 2.4 to the sun graph until the sun graph becomes the cycle C_n, it is proven that e^{χ} attains an extremal graph at C_n, with the corresponding maximum value being $e^{\chi}(G) \leq ne^{\frac{1}{2}}$.

The sum of the above two maximum values is $3e^{\frac{1}{2}} - 2e^{\frac{1}{\sqrt{2}}} > 0$, which implies that the exponential Randić index for a cycle graph is greater than the exponential Randić index for a tree graph.

It is not difficult to observe that as the number of edges increases, the maximum value of the exponential Randić index for quasi-tree graphs also increases. Furthermore, by Lemma 2.2, Lemma 2.3, Lemma 2.4, and Theorem 3.1, it can be concluded that when the number of edges is fixed, the quasi-tree graph achieves the maximum value of the exponential Randić index when $G - x \cong P_n$.

Therefore, when the number of edges is $2n-3$, the maximum value of the exponential Randić index is:

$$e^{\chi}(G) \leq 2e^{\frac{1}{\sqrt{2(n-1)}}} + (n+1)e^{\frac{1}{\sqrt{3(n-1)}}} + 2e^{\frac{1}{\sqrt{6}}} + (n-4)e^{\frac{1}{3}}.$$

The maximum value is attained if and only if $G - x$ belongs to P_n, and the equality holds if and only if $G = U_n^0$ (**Figure 2**).

3.2. The Lower Bounds and Extreme Graph

Theorem 3.2. Let G be a quasi-tree graph with n vertices and $n \geq 3$. Then, there exists:

$$e^{\chi}(G) \geq (n-3)e^{\frac{1}{\sqrt{n-1}}} + 2e^{\frac{1}{\sqrt{2(n-1)}}} + e^{\frac{1}{2}}$$

The equality holds if and only if $G \cong U_n^1$ (see **Figure 3**).

Proof. From the above conclusion, we can obtain that the exponential Randić index of a quasi-tree graph attains its maximum value at U_n^0. Moreover, as the number of edges in G decreases, the exponential Randić index may also decrease. Here, we do not consider the exponential Randić index of a tree graph. Therefore, we only need to consider the case where the number of edges is n, *i.e.*, when the quasi-tree graph is a cycle graph.

In the following proof, we assume that the graph G is a quasi-tree graph and we prove that $f(n) \leq e^{\chi}(G)$ holds if and only if $G \cong U_n^1$.

We proceed with mathematical induction on n. Since $G \in U_n^1$, it follows that $n \geq 4$. When $n = 4, 5$, the theorem holds (see **Figure 10**). In the following proof, we assume $G \in U_n^1$, where $n \geq 6$. Let M be the set of vertices in $V(G)$ with degree 1 (*i.e.*, $M = \{u \in V(G) \mid d(u) = 1\}$). Due to the previous conclusion, G is not a cycle graph, so M is not empty. Let $u \in M$ and let v be its neighbor, then $d(v) \geq 2$. Let $W(u) = \{y \mid y \in N(v) \setminus \{u\}, d(y) = 1\}$. Choose a vertex u_0 such that

1) The set $W(u_0)$ is as large as possible;

2) Under condition (1), $d(v)$ is as small as possible.

Let $G' = G - u_0$, then $G' \in \mathcal{U}_{n-1}$, $d(v) = d$ and $N_{G'}(v) = \{y_1, y_2, y_3, \cdots, y_{d-1}\}$. The e^{χ} value of all edges adjacent to v in G, except $u_0 v$, is denoted as S, and we can then obtain that,

$$S = \sum_{i=1}^{d-1} e^{\frac{1}{\sqrt{dd_{y_i}}}} .$$

Figure 10. The values of e^{χ} when $n = 4, 5$.

If $d(v)=3$ and $n=6,7,8$, there is

$$\left[(n-3)e^{\frac{1}{\sqrt{n-2}}}-(n-3)e^{\frac{1}{\sqrt{n-1}}}\right]+\left[2e^{\frac{1}{\sqrt{2(n-2)}}}-2e^{\frac{1}{\sqrt{2(n-1)}}}\right]+e^{\frac{1}{\sqrt{3}}}$$

$$-e^{\frac{1}{\sqrt{n-2}}}+e^{\frac{1}{\sqrt{3d_{y_1}}}}-e^{\frac{1}{\sqrt{2d_{y_1}}}}+e^{\frac{1}{\sqrt{3dd_2}}}-e^{\frac{1}{\sqrt{2dd_{y_2}}}}>0$$

The theorem has been proven to hold when the vertex degree is 2 or 3.

For the case of vertex degree greater than or equal to 4, we can deduce that there exists at least one vertex for which the graph *G*, when the vertex is removed, forms a subgraph *H* that is a tree with at least 2 vertices. This is because for all vertices *u* in *M*, there exists a vertex *u′* in *H* that is adjacent to *v′*, such that the degree of *v′* is 2 and $W(u)$ is not empty, which contradicts the premise. Therefore, the vertex degree $d(v)$ is not greater than 3.

For $d(y_1)=d(y_2)=\cdots=d(y_k)=1$, $(k\geq1)$ and $d(y_i)\geq2$. By Lemma 2.1, we can obtain,

$$S-S'=ke^{\frac{1}{\sqrt{d}}}+\sum_{i=k+1}^{d-1}e^{\frac{1}{\sqrt{dd_{y_i}}}}-ke^{\frac{1}{\sqrt{d-1}}}+\sum_{i=k+1}^{d-1}e^{\frac{1}{\sqrt{(d-1)d_{y_i}}}}$$

$$=k\left(e^{\frac{1}{\sqrt{d}}}-e^{\frac{1}{\sqrt{d-1}}}\right)+\sum_{i=k+1}^{d-1}e^{\frac{1}{\sqrt{dd_{y_i}}}}-\sum_{i=k+1}^{d-1}e^{\frac{1}{\sqrt{(d-1)d_{y_i}}}}$$

$$\geq k\left(e^{\frac{1}{\sqrt{d}}}-e^{\frac{1}{\sqrt{d-1}}}\right)+(d-1-k)\left(e^{\frac{1}{\sqrt{2d}}}-e^{\frac{1}{\sqrt{2(d-1)}}}\right)$$

Since $G\in U_n$, $k\leq d-2$, and $d(v)=d\leq n-2$. By Lemma 2.7, Lemma 2.8, we can obtain,

$$e^{\chi}(G)\geq f(n)+(n-4)e^{\frac{1}{\sqrt{n-2}}}+2e^{\frac{1}{\sqrt{2(n-2)}}}-(n-3)e^{\frac{1}{\sqrt{n-1}}}-2e^{\frac{1}{\sqrt{2(n-1)}}}+e^{\frac{1}{\sqrt{d}}}$$

$$+k\left(e^{\frac{1}{\sqrt{d}}}-e^{\frac{1}{\sqrt{d-1}}}\right)+(d-1-k)\left(e^{\frac{1}{\sqrt{2d}}}-e^{\frac{1}{\sqrt{2(d-1)}}}\right)$$

$$\geq f(n)+(n-4)e^{\frac{1}{\sqrt{n-2}}}+2e^{\frac{1}{\sqrt{2(n-2)}}}-(n-3)e^{\frac{1}{\sqrt{n-1}}}-2e^{\frac{1}{\sqrt{2(n-1)}}}+e^{\frac{1}{\sqrt{d}}}$$

$$+(d-2)\left(e^{\frac{1}{\sqrt{d}}}-e^{\frac{1}{\sqrt{d-1}}}\right)+\left(e^{\frac{1}{\sqrt{2d}}}-e^{\frac{1}{\sqrt{2(d-1)}}}\right)$$

$$\geq f(n)+(n-4)e^{\frac{1}{\sqrt{n-2}}}+2e^{\frac{1}{\sqrt{2(n-2)}}}-(n-3)e^{\frac{1}{\sqrt{n-1}}}-2e^{\frac{1}{\sqrt{2(n-1)}}}+e^{\frac{1}{\sqrt{n-2}}}$$

$$+(n-4)\left(e^{\frac{1}{\sqrt{n-2}}}-e^{\frac{1}{\sqrt{n-3}}}\right)+\left(e^{\frac{1}{\sqrt{2(n-2)}}}-e^{\frac{1}{\sqrt{2(n-3)}}}\right)$$

$$=f(n)+(n-3)\left(e^{\frac{1}{\sqrt{n-2}}}-e^{\frac{1}{\sqrt{n-1}}}\right)+(n-4)\left(e^{\frac{1}{\sqrt{n-2}}}-e^{\frac{1}{\sqrt{n-3}}}\right)$$

$$+2\left(e^{\frac{1}{\sqrt{2(n-2)}}}-e^{\frac{1}{\sqrt{2(n-1)}}}\right)+\left(e^{\frac{1}{\sqrt{2(n-2)}}}-e^{\frac{1}{\sqrt{2(n-3)}}}\right)$$

$$>f(n)$$

Proof completed.

4. Conclusion

In this paper, based on existing research results, we have studied the exponential Randić index. By using mathematical induction and various structural transformations of graphs, we have obtained extremal values and extremal graphs, and have got some new conclusions.

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Conflicts of Interest

The authors declare that they have no conflicts of interest to this work.

References

[1] Bollobás, B. and Erdös, P. (1998) Graphs of Extremal Weights. *Ars Combinatorial*, **50**, 225-233.

[2] Hu, Y.M., Li, X.L. and Yuan, Y. (2004) Trees with Minimum General Randić Index. *MATCH Communications in Mathematical and in Computer Chemistry*, **52**, 119-128.

[3] Li, X.L., Shi, Y.T. and Xu, T.Y. (2006) Unicyclic Graphs with Maximum General Randic Index for alpha> 0. *MATCH Communications in Mathematical and in Computer Chemistry*, **56**, 557-570.

[4] Wu, B.Y.D.R. and Zhang, L. (2005) Unicyclic Graphs with Minimum General Randic Index. *MATCH Communications in Mathematical and in Computer Chemistry*, **54**, 455-464.

[5] Pavlović, L. (2003) Maximal Value of the Zeroth-Order Randić Index. *Discrete Applied Mathematics*, **127**, 615-626. https://doi.org/10.1016/S0166-218X(02)00392-X

[6] Li, X.L. and Zhao, H.X. (2004) Trees with the First Three Smallest and Largest Generalized Topological Indices. *MATCH Communications in Mathematical and in Computer Chemistry*, **50**, 57-62.

[7] Zhang, S.G. and Zhang, H.L. (2006) Unicyclic Graphs with the First Three Smallest and Largest First General Zagreb Index. *MATCH Communications in Mathematical and in Computer Chemistry*, **55**, 427-438.

[8] Jahanbani, A., Cancan, M. and Motamedi, R. (2022) Extremal Trees for the Exponential of Forgotten Topological Index. *Journal of Mathematics*, **2022**, Article ID: 7455701. https://doi.org/10.1155/2022/7455701

[9] Lu, M. and Gao, J.W. (2007) On the Randić Index of Quasi-Tree Graphs. *Journal of Mathematical Chemistry*, **42**, 297-310. https://doi.org/10.1007/s10910-006-9089-6

[10] Sun, X.L., Gao, Y.B. and Du, J.W. (2022) The Zeroth-Order Generalized Randić Index of Quasi-Tree Graphs. *Journal of Shandong University* (*Natural Science*), **57**, 96-102.