

Research Paper

## ON THE MAXIMAL RANDIĆ ENERGY OF TREES WITH GIVEN DIAMETER

SHIVA SEPIDBON, NADER JAFARI RAD\* AND AKBAR JAHANBANI

**ABSTRACT.** For given integers  $n, d$  with  $n \geq 5$  and  $4 \leq d \leq n - 1$ , let  $T_d^n$  be the family of all trees of order  $n$  and diameter  $d$ . In this paper, we study trees  $T \in T_d^n$  with maximal Randić energy. We prove that if  $T \in T_d^n$  is a tree with maximal Randić energy then  $T$  is obtained from a path  $P = v_0v_1 \dots v_d$  by adding  $n_i$  path(s)  $P_3$  to each vertex  $v_i$ , for  $i = 2, 3, 4, \dots, d - 2$ , where  $n_i \in \{\lceil \frac{n-d+3}{2d-6} \rceil, \lfloor \frac{n-d+3}{2d-6} \rfloor\}$ . In particular, we present families of trees satisfying the Gutman-Furtula-Bozkurt Conjecture proposed in [Linear Algebra Appl., 442 (2014), 50–57].

### 1. INTRODUCTION

Let  $G = (V, E)$  be a graph with vertex set  $V = \{v_1, v_2, \dots, v_n\}$  and edge set  $E = E(G)$ , and let  $|V(G)| = n$  and  $|E(G)| = m$ . If the vertices  $v_i$  and  $v_j$  are adjacent, we write  $v_iv_j \in E(G)$ . For  $i = 1, 2, \dots, n$ , let  $d_{v_i} = d_G(v_i)$  be the degree of the vertex  $v_i$ . If  $d_{v_i} = 1$ , then  $v_i$  is a *pendant* vertex. A set of edges  $M$  of a graph  $G$  is a *matching* if no pair of edges of  $M$  share a

DOI: 10.22034/as.2023.20297.1654

MSC(2010): Primary: 05C50.

Keywords: Diameter, Randić index, Tree.

Received: 07 July 2023, Accepted: 08 November 2023.

\*Corresponding author

vertex. A matching of size  $k$  is referred as a  $k$ -*matching*. The *eccentricity* of a vertex  $v$  is the greatest distance from  $v$  to any other vertex of  $G$ . The *diameter* of a graph is the maximum over eccentricities of all vertices of the graph and is denoted by  $d$ . A *diametrical path* of a graph is the shortest path whose length is equal to the diameter of the graph.

For an integer  $p \geq 0$ , the tree  $S^p$  of order  $n = 2p + 1$ , containing  $p$  pendant vertices, each attached to a vertex of degree 2, and a vertex of degree  $p$ , is called the  $p$ -*sun*.

For integers  $p, q \geq 0$ , the tree  $DS^{p,q}$  of order  $n = 2(p + q + 1)$ , obtained from a  $p$ -sun and a  $q$ -sun, by connecting their central vertices, is called a  $(p, q)$ -*double sun*.

The *adjacency matrix*  $A = A(G)$  of a graph  $G$  is defined by its entries as  $a_{ij} = 1$  if  $v_i v_j \in E(G)$  and 0 otherwise. Let  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$  be *eigenvalues* of the adjacency matrix of  $G$ . According to the eigenvalues of the adjacency matrix, the *energy* of a graph is defined as

$$\mathcal{E} = \mathcal{E}(G) = \sum_{i=1}^n |\lambda_i|.$$

The concept of energy of a graph was first used by Gutman in chemistry to approximate  $\pi$ -*electron* energy, see([7], [8], [9]).

The *Randić matrix* is defined as  $r_{ij} = \frac{1}{\sqrt{d_{v_i} d_{v_j}}}$  if  $v_i v_j \in E(G)$  and 0 otherwise. The Randić matrix is real symmetric, so we can order its eigenvalues so that  $\rho_1 \geq \rho_2 \geq \dots \geq \rho_n$ . The *Randić energy* (see [3]) is defined as

$$\mathcal{E}_R(G) = \sum_{i=1}^n |\rho_i|.$$

Gutman, Furtula and Bozkurt presented the following conjecture in [6] about the connected graphs with maximal Randić energy.

**Conjecture 1.1** ([6]). *Let  $G$  be a connected graph on  $n$  vertices. Then*

$$\mathcal{E}_R(G) \leq \begin{cases} \mathcal{E}_R(S^p), & \text{if } n = 2p + 1 \text{ is odd,} \\ \mathcal{E}_R(DS^{p,q}), & \text{if } n = 2(p + q + 1) \text{ is even.} \end{cases}$$

Gao et al. in [5] presented the minimal Randić energy of trees with a given diameter. Gao in [4], showed that the generalized double suns of odd order satisfy Conjecture 1.1. The validity of Conjecture 1.1 over some other families of graphs is shown by Allem, Braga, Pastine and Molina, [1, 2].

Let  $T_d^n$  be the class of trees of order  $n$  with diameter  $4 \leq d \leq n - 1$ . Let  $T \in T_d^n$  and  $M_k(T)$  be the set of all  $k$ -matchings of  $T$ , for  $1 \leq k \leq \lfloor \frac{n}{2} \rfloor$ . For  $e = uv \in E(T)$  and  $\alpha_k = \{e_1, e_2, \dots, e_k\} \in M_k(T)$ , we denote  $R_T(e) = R_T(uv) = \frac{1}{d_T(u)d_T(v)}$ , and  $R_T(\alpha_k) =$

$\prod_{i=1}^k R_T(e_i)$ . The  $R$ -polynomial of  $T$  can be written as

$$\phi_R(T, x) = |xI - R(T)| = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k b(R(T), k) x^{n-2k},$$

where  $b(R(T), 0) = 1$  and  $b(R(T), k) = \sum_{\alpha_k \in M_k(T)} R_T(\alpha_k)$  for  $1 \leq k \leq \lfloor \frac{n}{2} \rfloor$  (see [10]).

**Theorem 1.2** ([10]). *Let  $T_1, T_2 \in T_d^n$ , and their  $R$ -polynomials be*

$$\phi_R(T_1, x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k b(R(T_1), k) x^{n-2k}, \quad \phi_R(T_2, x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k b(R(T_2), k) x^{n-2k},$$

*respectively. If  $b(R(T_1), k) \geq b(R(T_2), k)$  for all  $k \geq 1$ , and there is an integer number  $k$  such that  $b(R(T_1), k) > b(R(T_2), k)$ , then  $\mathcal{E}_R(T_1) > \mathcal{E}_R(T_2)$ .*

In this paper, we study trees with a given diameter and maximal Randić energy, therefore, we find families of graphs satisfying Conjecture 1.1. We prove for  $n \geq 5$  and  $4 \leq d \leq n - 1$ , if  $T \in T_d^n$  be a tree with maximal Randić energy then  $T$  is obtained from a path  $P = v_0 v_1 \dots v_d$  by adding  $n_i$  path(s)  $P_3$  to each vertex  $v_i$ , for  $i = 2, 3, 4, \dots, d-2$ , where  $n_i \in \{\lceil \frac{n-d+3}{2d-6} \rceil, \lfloor \frac{n-d+3}{2d-6} \rfloor\}$ .

## 2. OPERATIONS

In this section, we introduce some operations which are useful to obtain the maximum Randić energy trees of order  $n$  and diameter  $d$ . The following operations 1 and 5 were introduced in [5] and [11], respectively.

**Operation 1** ([5]). *Suppose that  $T$  is a tree, in addition, we assume that  $T_1$  is a subtree of  $T$ , such that  $v_1 \in V(T_1)$ ,  $t \geq 3$  and  $d_T(v_1) \geq 3$ . Define  $T' = T - \{v_1 v_3, v_1 v_4 \dots, v_1 v_t\} + \{v_2 v_3, v_3 v_4 \dots, v_{t-1} v_t\}$ . The above-referred graphs are illustrated in Figure 1.*

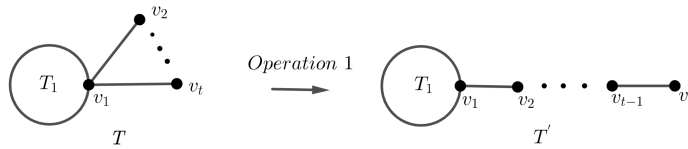
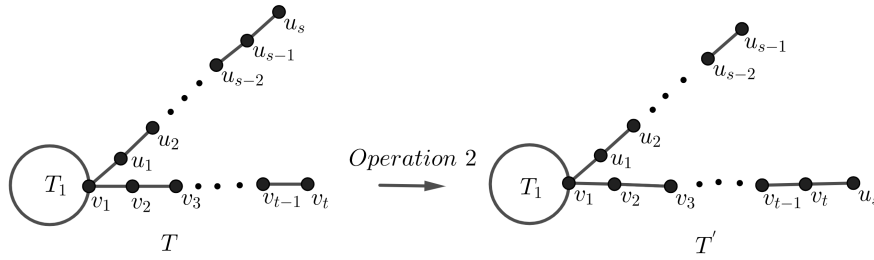


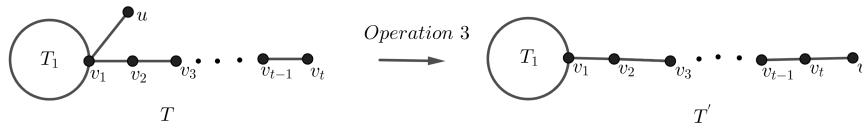
FIGURE 1. Trees  $T$  and  $T'$  for Operation 1.

We now present Operations 2, 3 and 4 as follows:

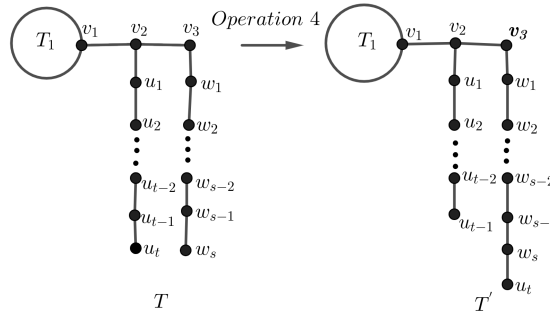
**Operation 2.** *Suppose that  $T$  is a tree, in addition, we assume that  $T_1$  is a subtree of  $T$ . Define  $T' = T - \{u_{s-1} u_s\} + \{v_t u_s\}$ . The above-referred trees are illustrated in Figure 2.*

FIGURE 2. Trees  $T$  and  $T'$  for Operation 2.

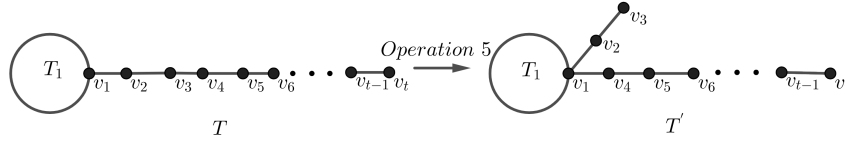
**Operation 3.** Suppose that  $T$  is a tree, in addition, we assume that  $T_1$  is a subtree of  $T$ , such that  $v_1 \in V(T_1)$  and  $d_T(v_1) \geq 3$ . Define  $T' = T - \{v_1 u\} + \{v_t u\}$ ,  $d_{T'}(v_1) \geq 2$ ,  $d_T(v_1) = d_{T'}(v_1) + 1$ . The above-referred trees are illustrated in Figure 3.

FIGURE 3. Trees  $T$  and  $T'$  for Operation 3.

**Operation 4.** Suppose that  $T$  is a tree and  $T_1$  is a subtree of  $T$ , such that  $v_1 \in V(T_1)$ . Define  $T' = T - \{u_{t-1} u_t\} + \{w_s u_t\}$ . The above-referred trees are illustrated in Figure 4.

FIGURE 4. Trees  $T$  and  $T'$  for Operation 4.

**Operation 5** ([11]). Suppose that  $T$  is a tree and  $T_1$  is a subtree of  $T$ , with  $v_1 \in V(T_1)$  such that  $d_T(v_1) \geq 2$ ,  $t \geq 7$ . Define  $T' = T - \{v_4 v_5 \dots v_t\} + \{v_1 v_4 v_5 \dots v_t\}$ . The above-referred trees are illustrated in Figure 5.

FIGURE 5. Trees  $T$  and  $T'$  for Operation 5.

### 3. USEFUL LEMMAS

In this section, we show that if a tree  $T'$  is obtained from a tree  $T$  by Operations 1, 2, 3, 4 and 5 then  $\mathcal{E}_R(T) \leq \mathcal{E}_R(T')$ . The following two lemmas corresponding to Operations 3.1 and 3.5 were presented in [5] and [11], respectively.

**Lemma 3.1** ([5]). *Let  $T$  and  $T'$  be two trees satisfying the conditions of Operation 1. Then  $\mathcal{E}_R(T) \leq \mathcal{E}_R(T')$ .*

We next present our lemmas for Operations 2, 3 and 4.

**Lemma 3.2.** *Let  $T$  and  $T'$  be two trees satisfying the conditions of Operation 2. Then  $\mathcal{E}_R(T) = \mathcal{E}_R(T')$ .*

*Proof.* Let the R-polynomials of  $T$  and  $T'$  be

$$\phi_R(T, x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k b(R(T), k) x^{n-2k}, \quad \phi_R(T', x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k b(R(T'), k) x^{n-2k},$$

respectively, where  $b(R(T), 0) = b(R(T'), 0) = 1$ . Then we have

$$\begin{aligned} b(R(T'), 1) - b(R(T), 1) &= R_{T'}(u_{s-2}u_{s-1}) + R_{T'}(v_{t-1}v_t) + R_{T'}(v_tu_s) \\ &\quad - R_T(u_{s-2}u_{s-1}) - R_T(u_{s-1}u_s) - R_T(v_{t-1}v_t) \\ &= \frac{1}{d_{T'}(u_{s-2})d_{T'}(u_{s-1})} + \frac{1}{d_{T'}(v_{t-1})d_{T'}(v_t)} + \frac{1}{d_{T'}(v_t)d_{T'}(u_s)} \\ &\quad - \frac{1}{d_T(u_{s-2})d_T(u_{s-1})} - \frac{1}{d_T(u_{s-1})d_T(u_s)} - \frac{1}{d_T(v_{t-1})d_T(v_t)} \\ &= \frac{1}{2} + \frac{1}{4} + \frac{1}{2} - \frac{1}{4} - \frac{1}{2} - \frac{1}{2} \\ &= 0. \end{aligned}$$

That is,  $b(R(T'), 1) = b(R(T), 1)$ .

For  $k = 2, \dots, \lfloor \frac{n}{2} \rfloor$ , we denote  $P_1 = v_1 u_1 u_2 \dots u_{s-2}$  and  $P_2 = v_1 v_2 \dots v_{t-1}$ , then we have

$$\begin{aligned}
b(R(T'), k) &= \sum_{\alpha_k \in M_k(T_1 \cup (p_1 \cup p_2))} R_{T'}(\alpha_k) \\
&+ \left( \frac{1}{d_{T'}(u_{s-2})d_{T'}(u_{s-1})} + \frac{1}{d_{T'}(v_t)d_{T'}(u_s)} \right) \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p_1 - u_{s-2}) \cup p_2)} R_{T'}(\alpha_{k-1}) \\
&+ \left( \frac{1}{d_{T'}(u_{s-2})d_{T'}(u_{s-1})} \times \frac{1}{d_{T'}(v_t)d_{T'}(u_s)} \right) \sum_{\alpha_{k-2} \in M_{k-2}(T_1 \cup (p_1 - u_{s-2}) \cup p_2)} R_{T'}(\alpha_{k-2}) \\
&+ \left( \frac{1}{d_{T'}(v_{t-1})d_{T'}(v_t)} + \frac{1}{d_{T'}(v_t)d_{T'}(u_s)} \right) \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup p_1 \cup (p_2 - v_{t-1}))} R_{T'}(\alpha_{k-1}) \\
&+ \left( \frac{1}{d_{T'}(u_{s-2})d_{T'}(u_{s-1})} + \frac{1}{d_{T'}(v_{t-1})d_{T'}(v_t)} \right) \\
&+ \left( \frac{1}{d_{T'}(v_t)d_{T'}(u_s)} \right) \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p_1 - u_{s-2}) \cup (p_2 - v_{t-1}))} R_{T'}(\alpha_{k-1}) \\
&+ \left( \frac{1}{d_{T'}(u_{s-2})d_{T'}(u_{s-1})} \times \frac{1}{d_{T'}(v_{t-1})d_{T'}(v_t)} \right) \\
&+ \left( \frac{1}{d_{T'}(u_{s-2})d_{T'}(u_{s-1})} \times \frac{1}{d_{T'}(v_t)d_{T'}(u_s)} \right) \sum_{\alpha_{k-2} \in M_{k-2}(T_1 \cup (p_1 - u_{s-2}) \cup (p_2 - v_{t-1}))} R_{T'}(\alpha_{k-2}) \\
&= \sum_{\alpha_k \in M_k(T_1 \cup (p_1 \cup p_2))} R_{T'}(\alpha_k) + \sum_{\alpha_{k-1} \in M_{k-1}(\mathcal{W}(p_1 - u_{s-2}) \cup p_2)} R_{T'}(\alpha_{k-1}) \\
&+ \frac{1}{4} \sum_{\alpha_{k-2} \in M_{k-2}(T_1 \cup (p_1 - u_{s-2}) \cup p_2)} R_{T'}(\alpha_{k-2}) + \frac{3}{4} \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup p_1 \cup (p_2 - v_{t-1}))} R_{T'}(\alpha_{k-1}) \\
&+ \frac{5}{4} \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p_1 - u_{s-2}) \cup (p_2 - v_{t-1}))} R_{T'}(\alpha_{k-1}) \\
&+ \frac{3}{8} \sum_{\alpha_{k-2} \in M_{k-2}(T_1 \cup (p_1 - u_{s-2}) \cup (p_2 - v_{t-1}))} R_{T'}(\alpha_{k-2}).
\end{aligned}$$

Similarly, we have

$$\begin{aligned}
b(R(T), k) &= \sum_{\alpha_k \in M_k(T_1 \cup (p_1 \cup p_2))} R_T(\alpha_k) \\
&+ \left( \frac{1}{d_T(u_{s-2})d_T(u_{s-1})} + \frac{1}{d_T(u_{s-1})d_T(u_s)} \right) \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p_1 - u_{s-2}) \cup p_2)} R_T(\alpha_{k-1}) \\
&+ \left( \frac{1}{d_T(u_{s-1})d_T(u_s)} + \frac{1}{d_T(v_{t-1})d_T(v_t)} \right) \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup p_1 \cup (p_2 - v_{t-1}))} R_T(\alpha_{k-1}) \\
&+ \left( \frac{1}{d_T(u_{s-1})d_T(u_s)} \times \frac{1}{d_T(v_{t-1})d_T(v_t)} \right) \sum_{\alpha_{k-2} \in M_{k-2}(T_1 \cup p_1 \cup (p_2 - v_{t-1}))} R_T(\alpha_{k-2})
\end{aligned}$$

$$\begin{aligned}
& + \left( \frac{1}{d_T(u_{s-2})d_T(u_{s-1})} + \frac{1}{d_T(u_{s-1})d_T(u_s)} \right. \\
& + \left. \frac{1}{d_T(v_{t-1})d_T(v_t)} \right) \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p_1 - u_{s-2}) \cup (p_2 - v_{t-1}))} R_T(\alpha_{k-1}) \\
& + \left( \frac{1}{d_T(u_{s-2})d_T(u_{s-1})} \times \frac{1}{d_T(v_{t-1})d_T(v_t)} \right. \\
& + \left. \frac{1}{d_T(u_{s-1})d_T(u_s)} \times \frac{1}{d_T(v_{t-1})d_T(v_t)} \right) \sum_{\alpha_{k-2} \in M_{k-2}(T_1 \cup (p_1 - u_{s-2}) \cup (p_2 - v_{t-1}))} R_T(\alpha_{k-2}) \\
& = \sum_{\alpha_k \in M_k(T_1 \cup (p_1 \cup p_2))} R_T(\alpha_k) + \frac{3}{4} \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p_1 - u_{s-2}) \cup p_2)} R_T(\alpha_{k-1}) \\
& + \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup p_1 \cup (p_2 - v_{t-1}))} R_T(\alpha_{k-1}) + \frac{1}{4} \sum_{\alpha_{k-2} \in M_{k-2}(T_1 \cup p_1 \cup (p_2 - v_{t-1}))} R_T(\alpha_{k-2}) \\
& + \frac{5}{4} \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p_1 - u_{s-2}) \cup (p_2 - v_{t-1}))} R_T(\alpha_{k-1}) + \frac{3}{8} \sum_{\alpha_{k-2} \in M_{k-2}(T_1 \cup (p_1 - u_{s-2}) \cup (p_2 - v_{t-1}))} R_T(\alpha_{k-2}).
\end{aligned}$$

since

$$\begin{aligned}
\sum_{\alpha_k \in M_k(T_1 \cup p_1 \cup p_2)} R_T(\alpha_k) &= \sum_{\alpha_k \in M_k(T_1 \cup p_1 \cup p_2)} R_{T'}(\alpha_k), \\
\sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup p_1 \cup (p_2 - v_{t-1}))} R_T(\alpha_{k-1}) &= \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p_1 - u_{s-2}) \cup p_2)} R_{T'}(\alpha_{k-1}), \\
\sum_{\alpha_{k-2} \in M_{k-2}(T_1 \cup p_1 \cup (p_2 - v_{t-1}))} R_T(\alpha_{k-2}) &= \sum_{\alpha_{k-2} \in M_{k-2}(T_1 \cup (p_1 - u_{s-2}) \cup p_2)} R_{T'}(\alpha_{k-2}), \\
\sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p_1 - u_{s-2}) \cup p_2)} R_T(\alpha_{k-1}) &= \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup p_1 \cup (p_2 - v_{t-1}))} R_{T'}(\alpha_{k-1}), \\
\sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p_1 - u_{s-2}) \cup (p_2 - v_{t-1}))} R_T(\alpha_{k-1}) &= \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p_1 - u_{s-2}) \cup (p_2 - v_{t-1}))} R_{T'}(\alpha_{k-1}), \\
\sum_{\alpha_{k-2} \in M_{k-2}(T_1 \cup (p_1 - u_{s-2}) \cup (p_2 - v_{t-1}))} R_T(\alpha_{k-2}) &= \sum_{\alpha_{k-2} \in M_{k-2}(T_1 \cup (p_1 - u_{s-2}) \cup (p_2 - v_{t-1}))} R_{T'}(\alpha_{k-2}),
\end{aligned}$$

it is easy to see that  $b(R(T'), k) - b(R(T), k) = 0$ . This implies  $b(R(T'), 1) = b(R(T), 1)$ . By Theorem 1.2, the lemma holds.  $\square$

**Lemma 3.3.** *Let  $T$  and  $T'$  be two trees satisfying the conditions of Operation 3. Then  $\mathcal{E}_R(T) \leq \mathcal{E}_R(T')$ .*

*Proof.* Let the R-polynomials of  $T$  and  $T'$  be

$$\phi_R(T, x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k b(R(T), k) x^{n-2k}, \quad \phi_R(T', x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k b(R(T'), k) x^{n-2k},$$

respectively, where  $b(R(T), 0) = b(R(T'), 0) = 1$ . Then we have

$$\begin{aligned}
b(R(T'), 1) - b(R(T), 1) &= R_{T'}(v_1 v_2) + R_{T'}(v_{t-1} v_t) + R_{T'}(v_t u) \\
&\quad - R_T(v_1 u) - R_T(v_1 v_2) - R_T(v_{t-1} v_t) \\
&= \frac{1}{d_{T'}(v_1) d_{T'}(v_2)} + \frac{1}{d_{T'}(v_{t-1}) d_{T'}(v_t)} + \frac{1}{d_{T'}(v_t) d_{T'}(u)} \\
&\quad - \frac{1}{d_T(v_1) d_T(u)} - \frac{1}{d_T(v_1) d_T(v_2)} - \frac{1}{d_T(v_{t-1}) d_T(v_t)} \\
&= \frac{1}{2d_{T'}(v_1)} + \frac{1}{4} + \frac{1}{2} - \frac{1}{d_T(v_1)} - \frac{1}{2d_T(v_1)} - \frac{1}{2} \\
&= \frac{1}{4} + \frac{1}{2d_{T'}(v_1)} - \frac{3}{2d_T(v_1)} > 0.
\end{aligned}$$

This implies  $b(R(T'), 1) > b(R(T), 1)$ .

For  $k = 2, \dots, \lfloor \frac{n}{2} \rfloor$ , we denote  $p = v_2 v_3 \dots v_{t-1}$ . Then

$$\begin{aligned}
b(R(T'), k) &= \sum_{\alpha_k \in M_k(T_1 \cup p)} R_{T'}(\alpha_k) + \frac{1}{d_{T'}(v_t) d_{T'}(u)} \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup p)} R_{T'}(\alpha_{k-1}) \\
&\quad + \frac{1}{d_{T'}(v_t) d_{T'}(u)} \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p-v_2))} R_{T'}(\alpha_{k-1}) \\
&\quad + \left( \frac{1}{d_{T'}(v_{t-1}) d_{T'}(v_t)} + \frac{1}{d_{T'}(v_t) d_{T'}(u)} \right) \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p-v_{t-1}))} R_{T'}(\alpha_{k-1}) \\
&\quad + \left( \frac{1}{d_{T'}(v_{t-1}) d_{T'}(v_t)} + \frac{1}{d_{T'}(v_t) d_{T'}(u)} \right) \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p-\{v_2, v_{t-1}\}))} R_{T'}(\alpha_{k-1}) \\
&= \sum_{\alpha_k \in M_k(T_1 \cup p)} R_{T'}(\alpha_k) + \frac{1}{2} \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup p)} R_{T'}(\alpha_{k-1}) \\
&\quad + \frac{1}{2} \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p-v_2))} R_{T'}(\alpha_{k-1}) + \frac{3}{4} \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p-v_{t-1}))} R_{T'}(\alpha_{k-1}) \\
&\quad + \frac{3}{4} \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p-\{v_2, v_{t-1}\}))} R_{T'}(\alpha_{k-1}).
\end{aligned}$$

Similarly, we have

$$\begin{aligned}
b(R(T), k) &= \sum_{\alpha_k \in M_k(T_1 \cup p)} R_T(\alpha_k) + \frac{1}{d_T(v_{t-1}) d_T(v_t)} \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup p-v_{t-1})} R_T(\alpha_{k-1}) \\
&\quad + \frac{1}{d_T(v_{t-1}) d_T(v_t)} \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p-\{v_2, v_{t-1}\}))} R_T(\alpha_{k-1}) \\
&= \sum_{\alpha_k \in M_k(T_1 \cup p)} R_T(\alpha_k) + \frac{1}{2} \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup p-v_{t-1})} R_T(\alpha_{k-1}) \\
&\quad + \frac{1}{2} \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p-\{v_2, v_{t-1}\}))} R_T(\alpha_{k-1}).
\end{aligned}$$



Note that

$$\begin{aligned}
\sum_{\alpha_k \in M_k(T_1 \cup p)} R_{T'}(\alpha_k) &= \sum_{\alpha_k \in M_k(T_1 \cup p)} R_T(\alpha_k), \\
\sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p-v_{t-1}))} R_{T'}(\alpha_{k-1}) &= \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p-v_{t-1}))} R_T(\alpha_{k-1}), \\
\sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p-\{v_2, v_{t-1}\}))} R_{T'}(\alpha_{k-1}) &= \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p-\{v_2, v_{t-1}\}))} R_T(\alpha_{k-1}),
\end{aligned}$$

So, we get

$$\begin{aligned}
b(R(T'), k) - b(R(T), k) &= \frac{1}{2} \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup p)} R_{T'}(\alpha_{k-1}) + \frac{1}{2} \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p-v_2))} R_{T'}(\alpha_{k-1}) \\
&\quad + \frac{1}{4} \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p-v_{t-1}))} R_{T'}(\alpha_{k-1}) \\
&\quad + \frac{1}{4} \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p-\{v_2, v_{t-1}\}))} R_{T'}(\alpha_{k-1}).
\end{aligned}$$

On the other hand, since

$$\begin{aligned}
\sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup p)} R_{T'}(\alpha_{k-1}) &\geq \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p-\{v_2, v_{t-1}\}))} R_{T'}(\alpha_{k-1}), \\
\sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p-v_2))} R_{T'}(\alpha_{k-1}) &\geq \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p-\{v_2, v_{t-1}\}))} R_{T'}(\alpha_{k-1}), \\
\sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p-v_{t-1}))} R_{T'}(\alpha_{k-1}) &\geq \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p-\{v_2, v_{t-1}\}))} R_{T'}(\alpha_{k-1}),
\end{aligned}$$

we get

$$b(R(T'), k) - b(R(T), k) \geq \frac{3}{2} \sum_{\alpha_{k-1} \in M_{k-1}(T_1 \cup (p-\{v_2, v_{t-1}\}))} R_{T'}(\alpha_{k-1}) > 0.$$

that is,  $b(R(T'), k) > b(R(T), k)$ . By Theorem 1.2, the lemma holds.  $\square$

**Lemma 3.4.** *Let  $T$  and  $T'$  be two trees satisfying the conditions of Operation 4. Then  $\mathcal{E}_R(T) = \mathcal{E}_R(T')$ .*

*Proof.* Let the R-polynomials of  $T$  and  $T'$  be

$$\phi_R(T, x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k b(R(T), k) x^{n-2k}, \quad \phi_R(T', x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k b(R(T'), k) x^{n-2k},$$

respectively, where  $b(R(T), 0) = b(R(T'), 0) = 1$ . Then we have

$$\begin{aligned}
 b(R(T'), 1) - b(R(T), 1) &= R_{T'}(u_{t-2}u_{t-1}) + R_{T'}(w_{s-1}w_s) + R_{T'}(w_su_t) \\
 &\quad - R_T(u_{t-2}u_{t-1}) - R_T(u_{t-1}u_t) - R_T(w_{s-1}w_s) \\
 &= \frac{1}{d_{T'}(u_{t-2})d_{T'}(u_{t-1})} + \frac{1}{d_{T'}(w_{s-1})d_{T'}(w_s)} + \frac{1}{d_{T'}(w_s)d_{T'}(u_t)} \\
 &\quad - \frac{1}{d_T(u_{t-2})d_T(u_{t-1})} - \frac{1}{d_T(u_{t-1})d_T(u_t)} - \frac{1}{d_T(w_{s-1})d_T(w_s)} \\
 &= \frac{1}{2} + \frac{1}{4} + \frac{1}{2} - \frac{1}{4} - \frac{1}{2} - \frac{1}{2} = 0.
 \end{aligned}$$

Thus the above equality is equivalent to  $b(R(T'), 1) = b(R(T), 1)$ .

For  $k = 2, \dots, \lfloor \frac{n}{2} \rfloor$ , we use  $p_1 = v_1v_2v_3$  and  $p_2 = v_2u_1u_2 \dots u_{t-2}$ ,  $p_3 = v_3w_1w_2 \dots w_{s-1}$ . By the same argument as lemma 3.2, we can prove that  $b(R(T'), k) = b(R(T), k)$ .  $\square$

In [11], the following lemma is proved.

**Lemma 3.5** ([11]). *Let  $T$  and  $T'$  be two trees satisfying the conditions of Operation 5. Then  $\mathcal{E}_R(T) \leq \mathcal{E}_R(T')$ .*

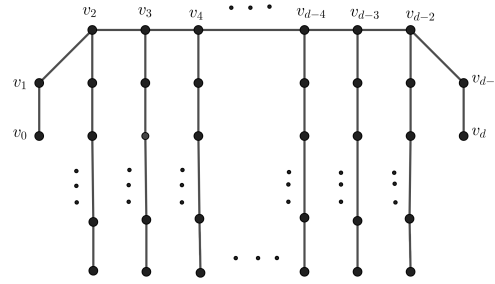
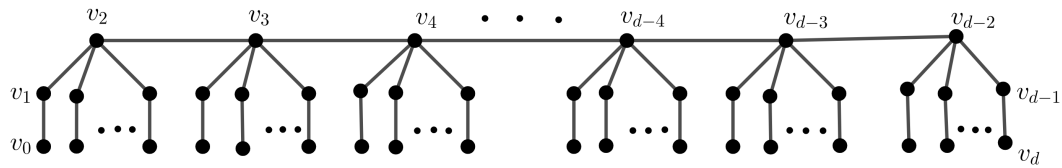
#### 4. MAIN RESULT

Let  $T(n_2, n_3, \dots, n_{d-2})$  be the class of trees  $T$  such that  $T$  is obtained from a path  $P = v_0v_1 \dots v_d$  by adding  $n_i$  path(s)  $P_3$  to each vertex  $v_i$ , for  $i = 2, 3, 4, \dots, d-2$ , where  $n_i \in \{\lceil \frac{n-d+3}{2d-6} \rceil, \lfloor \frac{n-d+3}{2d-6} \rfloor\}$ . Also, let  $T'(n_2, n_3, \dots, n_{d-2})$  be the class of trees  $T'$  such that  $T'$  is obtained from a tree  $T \in T(n_2, n_3, \dots, n_{d-2})$  by adding a leaf to one of the path(s)  $p_3$ .

**Theorem 4.1.** *Let  $T \in T_d^n$  be a tree with maximal Randić energy, where  $4 \leq d \leq n-1$  and  $n \geq 5$ . If  $n$  is odd and  $d$  is even or  $n$  is even and  $d$  is odd, then  $T \in T(n_2, n_3, \dots, n_{d-2})$ . If both  $n$  and  $d$  are odd or both  $n$  and  $d$  are even, then  $T \in T'(n_2, n_3, \dots, n_{d-2})$ .*

*Proof.* Let  $T \in T_d^n$  be a tree with maximal Randić energy, where  $4 \leq d \leq n-1$  and  $n \geq 5$ . We prove that if  $n$  is odd and  $d$  is even or  $n$  is even and  $d$  is odd, then there is a tree  $T' \in T(n_2, n_3, \dots, n_{d-2})$  such that  $\mathcal{E}_R(T) \leq \mathcal{E}_R(T')$ , and if both  $n$  and  $d$  are odd or both  $n$  and  $d$  are even, then there is a tree  $T' \in T'(n_2, n_3, \dots, n_{d-2})$  such that  $\mathcal{E}_R(T) \leq \mathcal{E}_R(T')$ . Let  $P = v_0v_1v_2 \dots v_d$  be a diametrical path in  $T$ . By Lemma 3.1, there is a tree  $T_1 \in T_d^n$  such that  $\mathcal{E}_R(T) \leq \mathcal{E}_R(T_1)$ . By Lemmas 3.2 and 3.3, there is a tree  $T_2 \in T_d^n$  such that  $\mathcal{E}_R(T_1) \leq \mathcal{E}_R(T_2)$ . Now, if there is a pendant vertex on the tree  $T_2$ , applying Operation 3, then there is a tree  $T_3 \in T_d^n$  as show in Figure 6 such that  $\mathcal{E}_R(T_2) \leq \mathcal{E}_R(T_3)$ .

Note that by Lemma 3.4 we have even number of vertices in each path connected to the diametrical path in Figure 6. Finally by Lemma 3.5 there is a tree  $T_4 \in T(n_2, n_3, \dots, n_{d-2})$  as shown in Figure 7 such that  $\mathcal{E}_R(T_3) \leq \mathcal{E}_R(T_4)$ .  $\square$

FIGURE 6. The tree  $T_3$ .FIGURE 7. The tree  $T_4$ .

As a consequence of Theorem 4.1, we obtain the following which proves the validity of Conjecture 1.1 for particular classes of trees.

**Corollary 4.2.** *Let  $T \in T_d^n$ . Then*

$$\mathcal{E}_R(T) \leq \begin{cases} \mathcal{E}_R(S^p) & \text{if } d=4 \text{ and } n=2p+1 \\ \mathcal{E}_R(DS^{p,q}) & \text{if } d=5 \text{ and } n=2(p+q+1). \end{cases}$$

## 5. CONCLUSION

In this paper, using Operations 1, 2, 3, 4 and 5 we have determined trees  $T \in T_d^n$  with maximal Randić energy. In particular, we presented families of trees satisfying Conjecture 1.1.

## REFERENCES

- [1] L. E. Allem, R. O. Braga and A. Pastine, *Randić index and energy*, MATCH Commun. Math. Comput. Chem., **83** (2020) 611-622.
- [2] L. E. Allem, G. Molina and A. Pastine, *Short note on Randić energy*, MATCH Commun. Math. Comput. Chem., **82** (2019) 515-528.
- [3] S. B. Bozkurt and D. Bozkurt, *Randić energy and Randić Estrada index of a graph*, Eur. J. Pure Appl. Math., **5** No. 1 (2012) 88-96.
- [4] W. Gao, *The Randić energy of generalized double sun*, Czech. Math. J., **92** No. 1 (2021) 285-312.

- [5] Y. Gao, W. Gao and Y. Shao, *The minimal Randić energy of trees with given diameter*, Appl. Math. Comput., **411** (2021) 126489.
- [6] I. Gutman, B. Furtula and S. B. Bozkurt, *On Randić energy*, Linear Algebra Appl., **442** (2014) 50-57.
- [7] I. Gutman and N. Trinajstić, *Graph theory and molecular orbitals. Total  $\pi$ -electron energy of alternant hydrocarbons*, Chem. Phys. Lett. **17** No. 4 (1972) 535-538.
- [8] I. Gutman and O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer, Berlin, 1986.
- [9] I. Gutman, *The Energy of a Graph: Old and New Results*, In: A. Betten, A. Kohnert, R. Laue and A. Wassermann (Eds.), Algebraic Combinatorics and Applications, Springer-Verlag, Berlin, 196-211, 2001.
- [10] J. He, Y. M. Liu and J. K. Tian, *Note on the Randić energy of graphs*, Kragujevac J. Math., **42** No. 2 (2018) 209-215.
- [11] X. Zhao, Y. Shao and Y. Gao, *On Randić energy of coral trees*, MATCH Commun. Math. Comput. Chem., **88** No. 1 (2022) 157-170.

**Shiva Sepidbon**

Department of Mathematics,

Shahed University,

Tehran, Iran.

`shiva.sepidbon@shahed.ac.ir`

**Nader Jafari Rad**

Department of Mathematics,

Shahed University,

Tehran, Iran.

`n.jafarirad@gmail.com`

**Akbar Jahanbani**

Department of Mathematics,

Azarbaijan Shahid Madani University,

Tabriz, Iran.

`akbarjahanbani92@gmail.com`