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Research Article

Extremal trees for the exponential reduced second Zagreb index

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Abstract

The reduced second Zagreb index $RM_2(G)$ of a graph G is defined as $RM_2(G) = \sum_{uv\in E(G)}(d_G(u)-1)(d_G(v)-1)$, where $d_G(u)$ and $d_G(v)$ are the degrees of vertices u and v, respectively. The exponential reduced second Zagreb index $e^{RM_2}(G)$ of G is defined as $e^{RM_2}(G) = \sum_{uv\in E(G)} e^{(d_G(u)-1)(d_G(v)-1)}$. In this paper, we determine the minimum and maximum exponential reduced second Zagreb index of (chemical) trees, and characterize the corresponding extremal graphs.

Keywords: extremal value; tree; chemical tree; exponential reduced second Zagreb index.

2020 Mathematics Subject Classification: 05C09, 05C35, 05C92.

1. Introduction

Chemical graph theory is a branch of mathematical chemistry. In chemical graph theory, graphs are used to represent compounds, in which vertices represent atoms and edges represent covalent bonds between atoms. In order to describe the structural properties of various molecules, mathematical chemists have introduced a variety of molecular descriptors (or topological indices). Topological indices are the numerical invariants that describe the structural characteristics of molecules. They are often used for the development of QSAR (Quantitative Structure-Activity Relationships) and QSPR (Quantitative Structure-Property Relationships). In recent years, topological indices have been widely used in the research of complex networks, such as biological networks, communication networks and social networks.

Let $G = (V(G), E(G))$ be a simple connected graph with its vertex set $V(G)$ and edge set $E(G)$. For a vertex $u \in V(G)$, the degree of u, denoted by $d_G(u)$ (or simply $d(u)$), is the number of vertices adjacent to u. Let r-vertex be a vertex of degree r. A tree having maximum vertex degree at most 4 is called a molecular tree or chemical tree. Denote by $\mathcal{T}_n$ (respectively, $\mathcal{C}_n$) the set of trees (respectively, chemical trees) with n vertices. Throughout this paper, undefined notations and terminologies can be found in [4].

The first Zagreb index (M_1) and the second Zagreb index (M_2) are among the most famous topological indices, and they are defined [16] as

$$M_1(G) = \sum_{v\in V(G)} (d_G(u))^2,$$

$$M_2(G) = \sum_{uv\in E(G)} d_G(u)d_G(v).$$

For details about M_1 and M_2, see [1–3, 12, 14, 15, 19, 22, 24].

The reduced second Zagreb index $RM_2(G)$ of graph G is defined [17] as

$$RM_2(G) = \sum_{uv\in E(G)} (d_G(u)-1)(d_G(v)-1).$$

For details about RM_2, see [5, 18, 20, 21, 26].

Recently, Rada [23] introduced the concept of exponential topological indices. Naturally, the exponential reduced second Zagreb index of graph G can be defined as

$$e^{RM_2}(G) = \sum_{uv\in E(G)} e^{(d_G(u)-1)(d_G(v)-1)}.$$

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Recently, the study of exponential topological indices caught some scholars' eyes. Cruz et al. [8,11] obtained extremal values of some exponential topological indices over trees and chemical trees. The same authors [9] determined the maximum ABC index and minimum exponential GA index of chemical trees. They [10] also obtained maximum exponential Randić index of trees. Zeng et al. [27] solved an open problem proposed by Cruz and Rada [11]; they showed that exponential second Zagreb index attains its maximum value for the balanced double star among trees. Some other recent investigations on this topic can be found in [6,7].

Motivated by the papers [6,13,27], we determine the minimum and maximum exponential reduced second Zagreb index of (chemical) trees, and characterize the extremal (chemical) trees.

In Section 2, we investigate (chemical) trees with the minimum exponential reduced second Zagreb index. Chemical trees with the maximum exponential reduced second Zagreb index are investigated in Section 3. In Section 4, we investigate trees with the maximum exponential reduced second Zagreb index and in Section 5 we conclude this paper.

2. (Chemical) Trees with the minimum exponential reduced second Zagreb index

In the following, we consider (chemical) trees with the minimum exponential reduced second Zagreb index. Note that

$$e^{RM_2}(T) = \sum_{uv\in E(T)} e^{(d_T(u)-1)(d_T(v)-1)} \geq \sum_{uv\in E(T)} e^0 = 2(n-1),$$

with equality if and only if $T \cong S_n$. Therefore, the star tree S_n has the minimum exponential reduced second Zagreb index among $\mathcal{T}_n$. Next, we only consider trees $T \ncong S_n$.

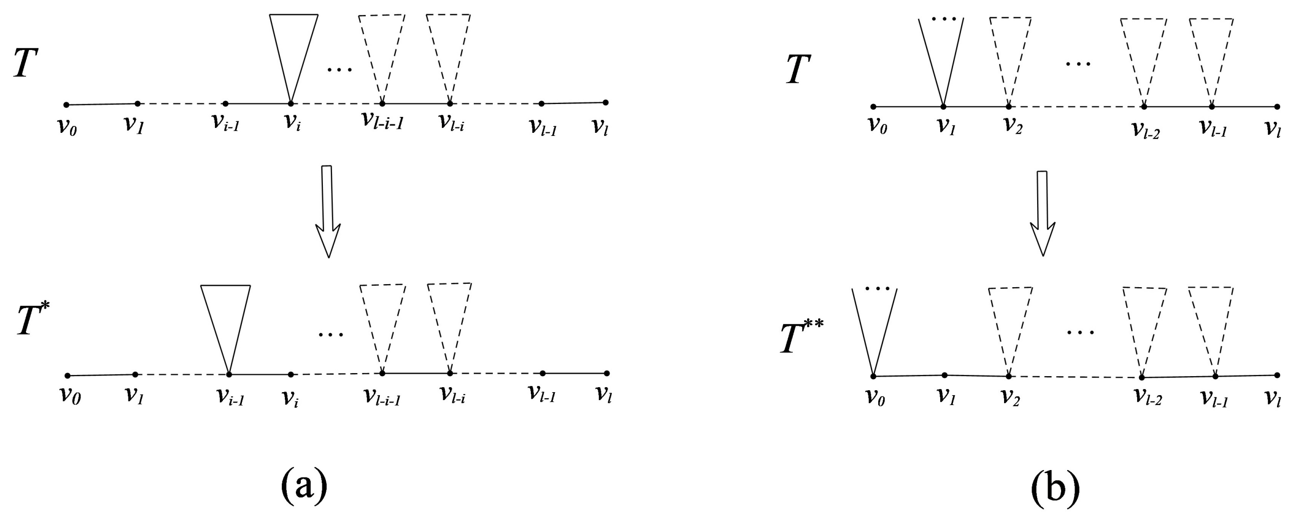

Figure 1: Transformations used in the proof of Theorem 2.1.

Theorem 2.1. *Let $T \in \mathcal{T}_n$ such that $T \ncong S_n$. Then, $e^{RM_2}(T) \geq e^{RM_2}(P_n)$ with equality if and only if $T \cong P_n$.*

Proof. Suppose that $T \in \mathcal{T}_n \setminus \{S_n\}$ is the minimal tree with respect to the exponential reduced second Zagreb index and let $v_0v_1v_2, \cdots, v_{l-1}v_l$ $(l \geq 3)$ be one of the longest paths in T. If $T \cong P_n$ then the conclusion holds. If $T \ncong P_n$ then there is a vertex of the longest path with neighbors not in the path. Without loss of generality, let i be the smallest index such that v_i has a neighbor not in the longest path. Let $d_i = d(v_i)$ for convenience.

Case 1: $i \geq 2$.
Suppose that $N_T(v_i) = \{v_{i-1}, v_{i+1}, v_{i_1}, v_{i_2} \cdots, v_{i_{d_i-2}}\}$. Let

$$T^* = T - \{v_iv_{i_1}, v_iv_{i_2}, \cdots, v_iv_{i_{d_i-2}}\} + \{v_{i-1}v_{i_1}, v_{i-1}v_{i_2}, \cdots, v_{i-1}v_{i_{d_i-2}}\},$$

see Figure 1(a). Note that $d_{i-2} \leq d_{i-1} = 2, d_{i+1} \geq 2, d_i \geq 3$. Then

$$\begin{aligned} e^{RM_2}(T^*) - e^{RM_2}(T) &= \left\{e^{(d_i-1)(d_{i-1}-1)} + e^{(d_i-1)(d_{i-2}-1)} + e^{(d_{i-1}-1)(d_{i+1}-1)}\right\} \\ &\quad - \left\{e^{(d_i-1)(d_{i-1}-1)} + e^{(d_i-1)(d_{i+1}-1)} + e^{(d_{i-2}-1)(d_{i-1}-1)}\right\} \\ &= \left\{e^{d_{i+1}-1} - e^{d_{i-2}-1}\right\} - \left\{e^{(d_i-1)(d_{i+1}-1)} - e^{(d_i-1)(d_{i-2}-1)}\right\} \\ &< 0. \end{aligned}$$

Case 2: $i = 1$.
Suppose that $N_T(v_1) = \{v_0, v_2, v_{1_1}, v_{1_2} \cdots, v_{1_{d_1-2}}\}$. Let $T^{**} = T - \{v_1v_{1_1}, v_1v_{1_2}, \cdots, v_1v_{1_{d_1-2}}\} + \{v_0v_{1_1}, v_0v_{1_2}, \cdots, v_0v_{1_{d_1-2}}\}$, see Figure 1(b). Note that $d_{i-2} \leq d_{i-1} = 2$, $d_{i+1} \geq 2$, and $d_i \geq 3$. Then,

$$\begin{aligned} e^{RM_2}(T^{**}) - e^{RM_2}(T) &= \left\{(d_1-2)e^0 + e^{d_1-2} + e^{d_2-1}\right\} - \left\{(d_1-1)e^0 + e^{(d_1-1)(d_2-1)}\right\} \\ &= e^{d_1-2} + e^{d_2-1} - e^{(d_1-1)(d_2-1)} - 1. \end{aligned}$$

Subcase 2.1: $d_2 = 2$.

$$\begin{aligned} e^{RM_2}(T^{**}) - e^{RM_2}(T) &= e^{d_1-2} + e^{d_2-1} - e^{(d_1-1)(d_2-1)} - 1 \\ &< 2e^{d_1-2} - e^{d_1-1} \\ &< 0. \end{aligned}$$

Subcase 2.2: $d_2 \geq 3$.
Suppose that $d_1 \geq d_2$. Since $d_1 \geq 3$ and $d_2 \geq 3$, it holds that

$$\begin{aligned} e^{RM_2}(T^{**}) - e^{RM_2}(T) &= e^{d_1-2} + e^{d_2-1} - e^{(d_1-1)(d_2-1)} - 1 \\ &< e^{d_1-1} + e^{d_2-1} - e^{(d_1-1)(d_2-1)} \\ &\leq 2e^{d_1-1} - e^{(d_1-1)(d_2-1)} \\ &< 2e^{d_1-1} - e^{2(d_1-1)} \\ &< 0. \end{aligned}$$

For $T \in \mathcal{T}_n \setminus \{S_n\}$, by using the transformations (a) and (b) of Figure 1 over and over again, we can finally obtain P_n. Thus, $e^{RM_2}(T) \geq e^{RM_2}(P_n)$ with equality if and only if $T \cong P_n$.

$\square$

By Theorem 2.1, we derive the following conclusion.

Corollary 2.1. *Let $T \in \mathcal{C}_n$ $(n \geq 6)$. Then $e^{RM_2}(T) \geq e^{RM_2}(P_n)$ with equality if and only if $T \cong P_n$.*

3. Chemical trees with the maximum exponential reduced second Zagreb index

In this section, we find the maximal chemical trees with respect to the exponential reduced second Zagreb index. These structures have some particular properties: (i) The number of 2-vertices is at most 1; (ii) The number of 3-vertices is at most 1; (iii) There do not exist both the 2-vertex and 3-vertex simultaneously. Denote by (n_1, n_2, n_3, n_4) the sequence of $T \in \mathcal{C}_n$ such that n_i is the number of vertices of T with degree i $(1 \leq i \leq 4)$. It is obvious that $e^{x+t} - e^x > e^{y+t} - e^y$ if $x > y$ and $t > 0$. This property will be frequently used in the upcoming lemmas.

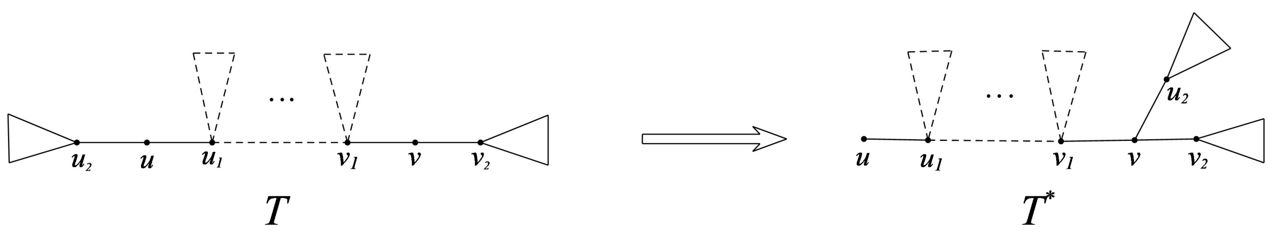

Figure 2: Transformation A used in Lemma 3.1.

Transformation A. Suppose that $T \in \mathcal{C}_n$ $(n \geq 5)$, and $d_T(u) = d_T(v) = 2$, $N_T(u) = \{u_1, u_2\}$, $N_T(v) = \{v_1, v_2\}$, $d_T(v_1) \geq d_T(u_1)$. Without loss of generality, we assume that the path between u and v contains u_1 and v_1. Note that if the path between u and v only has one edge, then $u = v_1$ and $v = u_1$. Let $T^* = T - uu_2 + vu_2$. These chemical trees are illustrated in Figure 2.

Lemma 3.1. *Let $T \in \mathcal{C}_n$ and $T^* \in \mathcal{C}_n$ $(n \geq 5)$ as shown in Figure 2. Then $e^{RM_2}(T^*) > e^{RM_2}(T)$.*

Proof. We proceed with the following two cases.

Case 1: $uv \notin E(T)$.
According to the definition of the exponential reduced second Zagreb index, we have

$$\begin{aligned} e^{RM_2}(T^*) - e^{RM_2}(T) &= \left\{e^{(d_{T^*}(v)-1)(d_{T^*}(u_2)-1)} + e^{(d_{T^*}(v)-1)(d_{T^*}(v_2)-1)} + e^{(d_{T^*}(v)-1)(d_{T^*}(v_1)-1)} + e^{(d_{T^*}(u)-1)(d_{T^*}(u_1)-1)}\right\} \\ &\quad - \left\{e^{(d_T(u)-1)(d_T(u_2)-1)} + e^{(d_T(v)-1)(d_T(v_2)-1)} + e^{(d_T(v)-1)(d_T(v_1)-1)} + e^{(d_T(u)-1)(d_T(u_1)-1)}\right\} \\ &= \left\{e^{2(d_T(u_2)-1)} + e^{2(d_T(v_2)-1)} + e^{2(d_T(v_1)-1)} + e^0\right\} - \left\{e^{(d_T(u_2)-1)} + e^{(d_T(v_2)-1)} + e^{(d_T(v_1)-1)} + e^{(d_T(u_1)-1)}\right\} \\ &\geq \left\{e^{2d_T(v_1)-2} - e^{d_T(v_1)-1}\right\} - \left\{e^{d_T(u_1)-1} - e^0\right\} \\ &\geq \left\{e^{d_T(u_1)-1+d_T(v_1)-1} - e^{d_T(v_1)-1}\right\} - \left\{e^{d_T(u_1)-1} - e^0\right\} \\ &> 0. \end{aligned}$$

Case 2: $uv \in E(T)$.
Since $n \geq 5$, we have $\min\{d_T(u_2), d_T(v_2)\} \geq 2$. Without loss of generality, we assume that $d_T(v_2) \geq 2$. Then,

$$\begin{aligned} e^{RM_2}(T^*) - e^{RM_2}(T) &= \left\{e^{(d_{T^*}(v)-1)(d_{T^*}(v_2)-1)} + e^{(d_{T^*}(v)-1)(d_{T^*}(u_2)-1)} + e^{(d_{T^*}(v)-1)(d_{T^*}(u)-1)}\right\} \\ &\quad - \left\{e^{(d_T(v)-1)(d_T(v_2)-1)} + e^{(d_T(u)-1)(d_T(u_2)-1)} + e^{(d_T(u)-1)(d_T(v)-1)}\right\} \\ &= \left\{e^{2(d_T(v_2)-1)} + e^{2(d_T(u_2)-1)} + e^0\right\} - \left\{e^{(d_T(v_2)-1)} + e^{(d_T(u_2)-1)} + e^1\right\} \\ &\geq \left\{e^{2d_T(v_2)-2} - e^{d_T(v_2)-1}\right\} - \left\{e^1 - e^0\right\} \\ &\geq \left\{e^{d_T(v_2)} - e^{d_T(v_2)-1}\right\} - \left\{e^1 - e^0\right\} \\ &> 0. \end{aligned}$$

□

From Lemma 3.1, we know that the number of 2-vertices of chemical trees with the maximum exponential reduced second Zagreb index is at most 1.

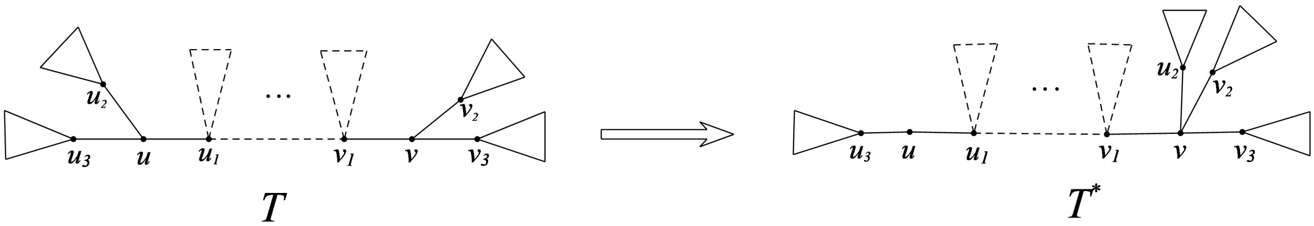

Figure 3: Transformation B used in Lemma 3.2.

Transformation B. Suppose that $T \in \mathcal{C}_n$ $(n \geq 7)$ and $d_T(u) = d_T(v) = 3$, $N_T(u) = \{u_1, u_2, u_3\}$, $N_T(v) = \{v_1, v_2, v_3\}$. Without loss of generality, we assume that the path between u and v contains u_1 and v_1. Note that if the path between u and v has only one edge, then $u = v_1$ and $v = u_1$. Let $T^* = T - uu_2 + vu_2$. These chemical trees are shown in Figure 3.

Lemma 3.2. *Let* $T \in \mathcal{C}_n$ *and* $T^* \in \mathcal{C}_n$ $(n \geq 7)$ *as shown in Figure 3. Then,* $e^{RM_2}(T^*) > e^{RM_2}(T)$.

Proof. We proceed by the following two cases.

Case 1: $uv \notin E(T)$.
Without loss of generality, we assume that $d_T(u_1) \leq d_T(v_1)$ and $d_T(u_3) \leq d_T(u_2)$, then

$$\begin{aligned} e^{RM_2}(T^*) - e^{RM_2}(T) &= \left\{e^{(d_{T^*}(u)-1)(d_{T^*}(u_3)-1)} + e^{(d_{T^*}(u)-1)(d_{T^*}(u_1)-1)} + e^{(d_{T^*}(v)-1)(d_{T^*}(v_1)-1)} + e^{(d_{T^*}(v)-1)(d_{T^*}(v_3)-1)}\right. \\ &\quad \left.+ e^{(d_{T^*}(v)-1)(d_{T^*}(v_2)-1)} + e^{(d_{T^*}(v)-1)(d_{T^*}(u_2)-1)}\right\} - \left\{e^{(d_T(u)-1)(d_T(u_2)-1)} + e^{(d_T(u)-1)(d_T(u_3)-1)}\right. \\ &\quad \left.+ e^{(d_T(u)-1)(d_T(u_1)-1)} + e^{(d_T(v)-1)(d_T(v_1)-1)} + e^{(d_T(v)-1)(d_T(v_2)-1)} + e^{(d_T(v)-1)(d_T(v_3)-1)}\right\} \\ &= \left\{e^{(d_T(u_3)-1)} + e^{(d_T(u_1)-1)} + e^{3(d_T(v_1)-1)} + e^{3(d_T(u_2)-1)} + e^{3(d_T(v_2)-1)} + e^{3(d_T(v_3)-1)}\right\} \\ &\quad - \left\{e^{2(d_T(u_2)-1)} + e^{2(d_T(u_3)-1)} + e^{2(d_T(u_1)-1)} + e^{2(d_T(v_1)-1)} + e^{2(d_T(v_2)-1)} + e^{2(d_T(v_3)-1)}\right\} \\ &\geq \left\{e^{3d_T(v_1)-3} - e^{2d_T(v_1)-2}\right\} + \left\{e^{3d_T(u_2)-3} - e^{2d_T(u_2)-2}\right\} \end{aligned}$$

$$
\begin{aligned}
&+\left\{e^{d_T(u_1)-1}-e^{2d_T(u_1)-2}\right\}+\left\{e^{d_T(u_3)-1}-e^{2d_T(u_3)-2}\right\}\\
&\geq \left\{e^{2d_T(v_1)-2+d_T(u_1)-1}-e^{2d_T(v_1)-2}\right\}-\left\{e^{2d_T(u_1)-2}-e^{d_T(u_1)-1}\right\}\\
&+\left\{e^{2d_T(u_2)-2+d_T(u_3)-1}-e^{2d_T(u_2)-2}\right\}-\left\{e^{2d_T(u_3)-2}-e^{d_T(u_3)-1}\right\}>0.
\end{aligned}
$$

Case 2: $uv \in E(T)$.

Without loss of generality, we assume $\max\{d_T(u_2), d_T(u_3), d_T(v_2), d_T(v_3)\} = d_T(v_3)$, then $d_T(v_3) \geq 2$ (since $n \geq 7$). Also, assume that $d_T(u_3) \leq d_T(u_2)$.

Subcase 2.1: $d_T(v_3) \geq 3$.

$$
\begin{aligned}
e^{RM_2}(T^*)-e^{RM_2}(T) &= \Big\{e^{(d_{T^*}(u)-1)(d_{T^*}(u_3)-1)}+e^{(d_{T^*}(v)-1)(d_{T^*}(u)-1)}+e^{(d_{T^*}(v)-1)(d_{T^*}(u_2)-1)}+e^{(d_{T^*}(v)-1)(d_{T^*}(v_2)-1)}\\
&\quad +e^{(d_{T^*}(v)-1)(d_{T^*}(v_3)-1)}\Big\}-\Big\{e^{(d_T(u)-1)(d_T(u_2)-1)}+e^{(d_T(u)-1)(d_T(u_3)-1)}+e^{(d_T(u)-1)(d_T(v)-1)}\\
&\quad +e^{(d_T(v)-1)(d_T(v_2)-1)}+e^{(d_T(v)-1)(d_T(v_3)-1)}\Big\}\\
&= \left\{e^{(d_T(u_3)-1)}+e^{3}+e^{3(d_T(u_2)-1)}+e^{3(d_T(v_2)-1)}+e^{3(d_T(v_3)-1)}\right\}\\
&\quad -\left\{e^{2(d_T(u_2)-1)}+e^{4}+e^{2(d_T(u_3)-1)}+e^{2(d_T(v_2)-1)}+e^{2(d_T(v_3)-1)}\right\}\\
&\geq \left\{e^{3d_T(v_3)-3}-e^{2d_T(v_3)-2}\right\}-\left\{e^{4}-e^{3}\right\}+\left\{e^{3d_T(u_3)-3}-e^{2d_T(u_2)-2}\right\}-\left\{e^{2d_T(u_3)-2}-e^{d_T(u_3)-1}\right\}\\
&\geq \left\{e^{2d_T(v_3)-1}-e^{2d_T(v_3)-2}\right\}-\left\{e^{4}-e^{3}\right\}+\left\{e^{d_T(u_3)-1+2d_T(u_2)-2}-e^{2d_T(u_2)-2}\right\}-\left\{e^{2d_T(u_3)-2}-e^{d_T(u_3)-1}\right\}\\
&> 0.
\end{aligned}
$$

Subcase 2.2: $d_T(v_3) = 2$.

Since $d_T(v_3) = 2$, let $N_T(v_3) = \{v, v_4\}$. Let $T^{**} = T - \{v_3v_4\} + \{vv_4\}$. Then

$$
\begin{aligned}
e^{RM_2}(T^{**})-e^{RM_2}(T) &= \Big\{e^{(d_{T^*}(v)-1)(d_{T^*}(u)-1)}+e^{(d_{T^*}(v)-1)(d_{T^*}(v_2)-1)}+e^{(d_{T^*}(v)-1)(d_{T^*}(v_3)-1)}+e^{(d_{T^*}(v)-1)(d_{T^*}(v_4)-1)}\Big\}\\
&\quad -\Big\{e^{(d_T(v)-1)(d_T(u)-1)}+e^{(d_T(v)-1)(d_T(v_2)-1)}+e^{(d_T(v)-1)(d_T(v_3)-1)}+e^{(d_T(v_4)-1)(d_T(v_3)-1)}\Big\}\\
&= \left\{e^{6}+e^{3(d_T(v_2)-1)}+e^{0}+e^{3(d_T(v_4)-1)}\right\}-\left\{e^{4}+e^{2(d_T(v_2)-1)}+e^{2}+e^{(d_T(v_4)-1)}\right\}\\
&\geq \left\{e^{6}-e^{4}\right\}-\left\{e^{2}-e^{0}\right\}\\
&> 0.
\end{aligned}
$$

□

By Lemma 3.2, we know that the number of 3-vertices of chemical trees with the maximum exponential reduced second Zagreb index is at most 1.

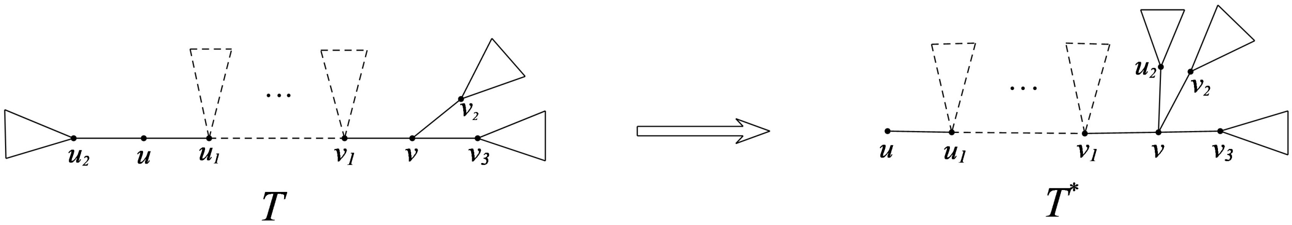

Figure 4: Transformation C used in Lemma 3.3.

Transformation C. Suppose that $T \in \mathcal{C}_n$ ($n \geq 7$) and $d_T(u) = 2$, $d_T(v) = 3$, $N_T(u) = \{u_1, u_2\}$, $N_T(v) = \{v_1, v_2, v_3\}$. Without loss of generality, we assume that the path between u and v contains u_1 and v_1. Note that if the path between u and v has only one edge, then $u = v_1$ and $v = u_1$. Let $T^* = T - uu_2 + vu_2$. These chemical trees are illustrated in Figure 4.

Lemma 3.3. *Let $T \in \mathcal{C}_n$ and $T^* \in \mathcal{C}_n$ $(n \geq 7)$ as shown in Figure 4. Then $e^{RM_2}(T^*) > e^{RM_2}(T)$.*

Proof. We consider the following two cases.

Case 1: $uv \notin E(T)$.
By Lemma 3.1 (Lemma 3.2, respectively), the number of 2-vertices (3-vertices, respectively) of chemical trees with the maximum exponential reduced second Zagreb index is at most 1. Thus, $d_T(u_1) = d_T(v_1) = 4$. Then

$$\begin{aligned}
e^{RM_2}(T^*) - e^{RM_2}(T) &= \Big\{e^{(d_{T^*}(u)-1)(d_{T^*}(u_1)-1)} + e^{(d_{T^*}(v)-1)(d_{T^*}(v_1)-1)} + e^{(d_{T^*}(v)-1)(d_{T^*}(v_2)-1)} + e^{(d_{T^*}(v)-1)(d_{T^*}(v_3)-1)} \\
&\quad + e^{(d_{T^*}(v)-1)(d_{T^*}(u_2)-1)}\Big\} - \Big\{e^{(d_T(u)-1)(d_T(u_1)-1)} + e^{(d_T(u)-1)(d_T(u_2)-1)} + e^{(d_T(v)-1)(d_T(v_1)-1)} \\
&\quad + e^{(d_T(v)-1)(d_T(v_2)-1)} + e^{(d_T(v)-1)(d_T(v_3)-1)}\Big\} \\
&= \Big\{e^0 + e^9 + e^{3(d_T(v_2)-1)} + e^{3(d_T(v_3)-1)} + e^{3(d_T(u_2)-1)}\Big\} \\
&\quad - \Big\{e^3 + e^6 + e^{(d_T(u_2)-1)} + e^{2(d_T(v_2)-1)} + e^{2(d_T(v_3)-1)}\Big\} \\
&\geq \{e^9 - e^6\} - \{e^3 - e^0\} \\
&> 0.
\end{aligned}$$

Case 2: $uv \in E(T)$.
Since $n \geq 7$, we have $\max\{d_T(u_2), d_T(v_2), d_T(v_3)\} \geq 2$. Without loss of generality, we assume that $d_T(v_2) \geq 2$. By Lemma 3.1 (Lemma 3.2, respectively), the number of 2-vertices (3-vertices, respectively) of chemical trees with the maximum exponential reduced second Zagreb index is at most 1. Thus $d_T(v_2) = 4$. Then

$$\begin{aligned}
e^{RM_2}(T^*) - e^{RM_2}(T) &= \Big\{e^{(d_{T^*}(v)-1)(d_{T^*}(u)-1)} + e^{(d_{T^*}(v)-1)(d_{T^*}(u_2)-1)} + e^{(d_{T^*}(v)-1)(d_{T^*}(v_2)-1)} + e^{(d_{T^*}(v)-1)(d_{T^*}(v_3)-1)}\Big\} \\
&\quad - \Big\{e^{(d_T(u)-1)(d_T(u_2)-1)} + e^{(d_T(v)-1)(d_T(u)-1)} + e^{(d_T(v)-1)(d_T(v_2)-1)} + e^{(d_T(v)-1)(d_T(v_3)-1)}\Big\} \\
&= \Big\{e^0 + e^{3(d_T(u_2)-1)} + e^{3(d_T(v_2)-1)} + e^{3(d_T(v_3)-1)}\Big\} \\
&\quad - \Big\{e^2 + e^{(d_T(u)-1)} + e^{2(d_T(v_2)-1)} + e^{2(d_T(v_3)-1)}\Big\} \\
&\geq \{e^9 - e^6\} - \{e^2 - e^0\} \\
&> 0.
\end{aligned}$$

□

By Lemma 3.3, we know that there do not exist both the 2-vertex and 3-vertex simultaneously in chemical trees with the maximum exponential reduced second Zagreb index. By Lemma 3.1, if $T \in \mathcal{C}_n$ with the sequence (n_1, n_2, n_3, n_4), there exists $T^* \in \mathcal{C}_n$ such that $e^{RM_2}(T^*) > e^{RM_2}(T)$ where the sequence of T^* is

$$\begin{cases} (n_1 + k, 0, n_3 + k, n_4) & \text{if } n_2 = 2k, \\ (n_1 + k, 1, n_3 + k, n_4) & \text{if } n_2 = 2k + 1. \end{cases}$$

By Lemma 3.3, if $T^* \in \mathcal{C}_n$ with vertex sequence $(n_1 + k, 1, n_3 + k, n_4)$ $(n_3 + k \geq 1)$ then by using Transformation C, there exists $T^{**} \in \mathcal{C}_n$ such that $e^{RM_2}(T^{**}) > e^{RM_2}(T^*)$, where the sequence of T^{**} is $(n_1 + k + 1, 0, n_3 + k - 1, n_4 + 1)$. Thus, we have the following result.

Lemma 3.4. *Let $T \in \mathcal{C}_n$ $(n \geq 7)$ with sequence (n_1, n_2, n_3, n_4), then there exists $T^* \in \mathcal{C}_n$ such that $e^{RM_2}(T^*) > e^{RM_2}(T)$ where T^* has the sequence*

$$\begin{cases} (n_1 + \frac{n_2}{2}, 0, n_3 + \frac{n_2}{2}, n_4) & \textit{if } n_2 \equiv 0 \pmod 2, \\ (n_1 + \frac{n_2+1}{2}, 0, n_3 + \frac{n_2-3}{2}, n_4 + 1) & \textit{if } n_2 \equiv 1 \pmod 2. \end{cases}$$

If $T \in \mathcal{C}_n$ with the sequence $(n_1, 0, n_3, n_4)$ $(n_3 \geq 2)$ then by Lemma 3.2, there exists $T^* \in \mathcal{C}_n$ with the sequence $(n_1, 1, n_3 - 2, n_4 + 1)$ such that $e^{RM_2}(T^*) > e^{RM_2}(T)$. If $n_3 - 2 \geq 1$, by Lemma 3.3, there exists $T^{**} \in \mathcal{C}_n$ with the sequence $(n_1 + 1, 0, n_3 - 3, n_4 + 1)$ such that $e^{RM_2}(T^{**}) > e^{RM_2}(T^*)$. Next, if $n_3 - 3 \geq 2$, by Lemma 3.2, there exists $T^{***} \in \mathcal{C}_n$ with the sequence $(n_1 + 1, 1, n_3 - 5, n_4 + 2)$ such that $e^{RM_2}(T^{***}) > e^{RM_2}(T^{**})$. Thus, using Transformations A, B, and C, repeatedly, we have the following result.

Lemma 3.5. *Let $T \in \mathcal{C}_n$ $(n \geq 7)$ with the sequence $(n_1, 0, n_3, n_4)$, then there exists $T^* \in \mathcal{C}_n$ such that $e^{RM_2}(T^*) > e^{RM_2}(T)$ where T^* has the sequence*

$$\begin{cases} (n_1 + \frac{n_3}{3}, 0, 0, n_4 + \frac{2n_3}{3}) & \textit{if } n_3 \equiv 0 \pmod 3, \\ (n_1 + \frac{n_3-1}{3}, 0, 1, n_4 + \frac{2n_3-2}{3}) & \textit{if } n_3 \equiv 1 \pmod 3, \\ (n_1 + \frac{n_3-2}{3}, 1, 0, n_4 + \frac{2n_3-1}{3}) & \textit{if } n_3 \equiv 2 \pmod 3. \end{cases}$$

For a chemical tree, one knows that $n = n_1 + n_2 + n_3 + n_4$ and $2(n-1) = n_1 + 2n_2 + 3n_3 + 4n_4$. Thus, $n = 2 + n_2 + 2n_3 + 3n_4$. By Lemma 3.4 and Lemma 3.5, we have the following result.

Lemma 3.6. *Let $T \in \mathcal{C}_n$ $(n \geq 7)$ with the sequence (n_1, n_2, n_3, n_4), then there exists $T^* \in \mathcal{C}_n$ such that $e^{RM_2}(T^*) > e^{RM_2}(T)$ where T^* has the sequence*

$$\begin{cases} (n_1, 1, 0, n_4) & \textit{if } n \equiv 0 \pmod 3, \\ (n_1, 0, 1, n_4) & \textit{if } n \equiv 1 \pmod 3, \\ (n_1, 0, 0, n_4) & \textit{if } n \equiv 2 \pmod 3. \end{cases}$$

In the following, we derive the maximum exponential reduced second Zagreb index of chemical tree $\mathcal{C}_n$.

Theorem 3.1. *Let $T \in \mathcal{C}_n$ $(n \geq 7)$, then*

$$e^{RM_2}(T) \leq \begin{cases} \frac{1}{3}(n-6)e^9 + e^3 + \frac{2}{3}n & \textit{if } n \equiv 0 \pmod 3, \\ \frac{1}{3}(n-7)e^9 + e^6 + \frac{1}{3}(2n+1) & \textit{if } n \equiv 1 \pmod 3, \\ \frac{1}{3}(n-5)e^9 + \frac{1}{3}(2n+2) & \textit{if } n \equiv 2 \pmod 3. \end{cases}$$

Proof. If $T \in \mathcal{C}_n$ then

$$e^{RM_2}(T) = \sum_{uv \in E(T)} e^{(d_T(u)-1)(d_T(v)-1)} = m_{12} + m_{13} + m_{14} + m_{22}e + m_{23}e^2 + m_{24}e^3 + m_{33}e^4 + m_{34}e^6 + m_{44}e^9.$$

Suppose that $T^* \in \mathcal{C}_n$ has the maximum exponential reduced second Zagreb index.

Case 1: $n \equiv 0 \pmod 3$.
By Lemma 3.6, T^* has the sequence $(n_1, 1, 0, n_4)$. Since $n = 2 + n_2 + 2n_3 + 3n_4$ and $n = n_1 + n_2 + n_3 + n_4$, we have $n_4 = \frac{n}{3} - 1$ and $n_1 = \frac{2n}{3}$. Since T^* has only one 2-vertex and has no 3-vertex, we proceed with the following two subcases.

Subcase 1.1: $m_{12} = 0$.
In this case, we have $m_{24} = 2$, $m_{44} = \frac{n}{3} - 3$, $m_{14} = \frac{2n}{3}$ and hence $e^{RM_2}(T^*) = m_{44}e^9 + m_{24}e^3 + m_{14} = \frac{1}{3}(n-9)e^9 + 2e^3 + \frac{2n}{3}$.

Subcase 1.2: $m_{12} = 1$.
We have $m_{24} = 1$, $m_{44} = \frac{n}{3} - 2$, $m_{12} = 1$, $m_{14} = \frac{2n}{3} - 1$ which imply $e^{RM_2}(T^*) = m_{44}e^9 + m_{24}e^3 + m_{12} + m_{14} = \frac{1}{3}(n-6)e^9 + e^3 + \frac{2n}{3}$.

Case 2: $n \equiv 1 \pmod 3$.
By Lemma 3.6, T^* has the sequence $(n_1, 0, 1, n_4)$. Since $n = 2 + n_2 + 2n_3 + 3n_4$ and $n = n_1 + n_2 + n_3 + n_4$, we have $n_4 = \frac{n-4}{3}$ and $n_1 = \frac{2n+1}{3}$. Since T^* has only one 3-vertex and has no 2-vertex, we can proceed with the following three subcases.

Subcase 2.1: $m_{13} = 0$.
Then $m_{34} = 3$, $m_{14} = \frac{2n+1}{3}$, $m_{44} = \frac{n-13}{3}$ and $e^{RM_2}(T^*) = m_{44}e^9 + m_{34}e^6 + m_{14} = \frac{1}{3}(n-13)e^9 + 3e^6 + \frac{1}{3}(2n+1)$.

Subcase 2.2: $m_{13} = 1$.
Then $m_{34} = 2$, $m_{44} = \frac{1}{3}(n-10)$, $m_{13} = 1$, $m_{14} = \frac{1}{3}(2n-2)$ and

$$e^{RM_2}(T^*) = m_{44}e^9 + m_{34}e^6 + m_{13} + m_{14} = \frac{1}{3}(n-10)e^9 + 2e^6 + \frac{1}{3}(2n+1).$$

Subcase 2.3: $m_{13} = 2$.
Then $m_{34} = 1$, $m_{44} = \frac{1}{3}(n-7)$, $m_{13} = 2$, $m_{14} = \frac{1}{3}(2n-5)$ and $e^{RM_2}(T^*) = m_{44}e^9 + m_{34}e^6 + m_{13} + m_{14} = \frac{1}{3}(n-7)e^9 + e^6 + \frac{1}{3}(2n+1)$.

Case 3: $n \equiv 2 \pmod 3$.
By Lemma 3.6, T^* has the sequence $(n_1, 0, 0, n_4)$. Since $n = 2 + n_2 + 2n_3 + 3n_4$ and $n = n_1 + n_2 + n_3 + n_4$, we have $n_4 = \frac{1}{3}(n-2)$ and $n_1 = \frac{2n+2}{3}$. Since T^* has no 2-vertex and has no 3-vertex, we get $m_{14} = \frac{1}{3}(2n+2)$, $m_{44} = \frac{1}{3}(n-5)$ and

$$e^{RM_2}(T^*) = m_{44}e^9 + m_{14} = \frac{1}{3}(n-5)e^9 + \frac{1}{3}(2n+2).$$

In summary, we complete the proof. □

4. Trees with the maximum exponential reduced second Zagreb index

In the following, we derive some properties of the tree with the maximum exponential reduced second Zagreb index.

Transformation D. Let $T \in \mathcal{T}_n$. Suppose that u_Δ is a vertex with the maximum degree and there exist one pendent vertex u_p such that $d_T(u_\Delta, u_p) \geq 3$. Then, there exist a path $P = u_\Delta vw$ from u_Δ to u_p such that $d_T(w) \geq 2$. Let $d_T(v) = k$, $d_T(w) = l$ and $N_T(v) = \{u_\Delta, w, v_1, v_2, \cdots, v_{k-2}\}$, $N_T(w) = \{v, w_1, w_2, \cdots, w_{l-1}\}$. Let

$$T^* = T - \{ww_1, ww_2, \cdots, ww_{l-1}\} + \{vw_1, vw_2, \cdots, vw_{l-1}\}.$$

Lemma 4.1. *Let $T \in \mathcal{T}_n$ and $T^* \in \mathcal{T}_n$ as defined above. Then, $e^{RM_2}(T^*) > e^{RM_2}(T)$.*

Proof. According to the definition of the exponential reduced second Zagreb index, we have

$$\begin{aligned}
e^{RM_2}(T^*) - e^{RM_2}(T) &= \left\{ e^{(\Delta-1)(k+l-2)} + \sum_{i=1}^{k-2} e^{(d_T(v_i)-1)(k+l-2)} + \sum_{i=1}^{l-1} e^{(d_T(w_i)-1)(k+l-2)} + e^0 \right\} \\
&\quad - \left\{ e^{(\Delta-1)(k-1)} + \sum_{i=1}^{k-2} e^{(d_T(v_i)-1)(k-1)} + \sum_{i=1}^{l-1} e^{(d_T(w_i)-1)(l-1)} + e^{(k-1)(l-1)} \right\} \\
&= e^{(\Delta-1)(k+l-2)} + e^0 - e^{(\Delta-1)(k-1)} - e^{(k-1)(l-1)} \\
&\quad + \sum_{i=1}^{k-2} (e^{(d_T(v_i)-1)(k+l-2)} - e^{(d_T(v_i)-1)(k-1)}) + \sum_{i=1}^{l-1} (e^{(d_T(w_i)-1)(k+l-2)} - e^{(d_T(w_i)-1)(l-1)}) \\
&\geq e^{(\Delta-1)(k+l-2)} + e^0 - 2e^{(\Delta-1)(k-1)} \\
&> e^{(\Delta-1)(k+l-2)} - e^{(\Delta-1)(k-1)+1} \\
&> 0.
\end{aligned}$$

□

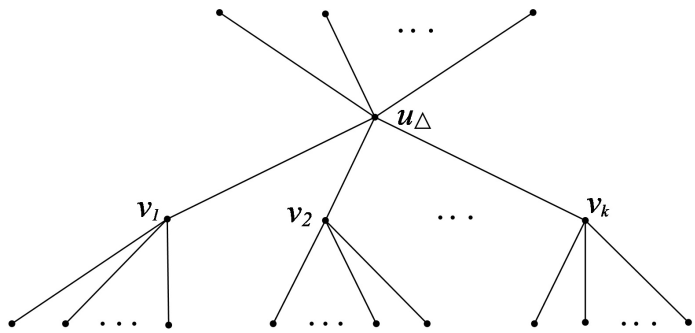

Figure 5: The structure of $T \in \mathcal{T}_n$ with the maximum exponential reduced second Zagreb index.

By Lemma 4.1, if $T \in \mathcal{T}_n$ with the maximum e^{RM_2} index, then $d_T(u_\Delta, u_p) \leq 2$. The tree T is shown in Figure 5. If $k = 1$ then T is a double star tree. If $k \geq 2$, then u_Δ is the only vertex of T with the maximum degree.

Transformation E. Suppose that $T_1 \in \mathcal{T}_{n-k-l-2}$ and u_Δ is the maximum degree vertex of T_1. Let S_1 be the star graph with $k+1$ vertices such that v is the center vertex and its pendent vertices are $v_1, v_2, \cdots, v_k$. Let S_2 be the star graph with $l+1$ vertices such that w is the center vertex and its pendent vertices are $w_1, w_2, \cdots, w_l$. Let $k \geq l \geq 1$. The graph $T \in \mathcal{T}_n$ is obtained from T_1, S_1, S_2 by connecting the vertices u and v, and the vertices u and w. Let $T^* = T - \{ww_1\} + \{vw_1\}$.

Lemma 4.2. *Let $T \in \mathcal{T}_n$ and $T^* \in \mathcal{T}_n$ as defined above. Then, $e^{RM_2}(T^*) > e^{RM_2}(T)$.*

Proof. According to the definition of the exponential reduced second Zagreb index, we have

$$\begin{aligned}
e^{RM_2}(T^*) - e^{RM_2}(T) &= \left\{ e^{(\Delta-1)(k+l)} + (k+1)e^0 + e^{(\Delta-1)(l-1)} + (l-1)e^0 \right\} - \left\{ e^{(\Delta-1)k} + ke^0 + e^{(\Delta-1)l} + le^0 \right\} \\
&= \left\{ e^{(\Delta-1)(k+l)} - e^{(\Delta-1)k} \right\} - \left\{ e^{(\Delta-1)(l-1)} - e^{(\Delta-1)l} \right\} \\
&= (e^{(\Delta-1)k} - e^{(\Delta-1)(l-1)})(e^{(\Delta-1)} - 1) \\
&> 0.
\end{aligned}$$

□

Lemma 4.3. *Let $T \cong S_{a,b}$ be the double star tree with n vertices, where $n = a+b+2$ and $a \geq b+2$. Let $T^* \cong S_{a-1,b+1}$. Then, $e^{RM_2}(T^*) > e^{RM_2}(T)$.*

Proof. According to the structure of the double star tree and the definition of the exponential reduced second Zagreb index, we have

$$\begin{aligned} e^{RM_2}(T^*) - e^{RM_2}(T) &= \left\{e^{(a-1)(b+1)} + (a-1)e^0 + (b+1)e^0\right\} - \left\{e^{ab} + ae^0 + be^0\right\} \\ &= e^{(a-1)(b+1)} - e^{ab} \\ &= e^{ab+a-b-1} - e^{ab} \\ &> 0. \end{aligned}$$

□

By Lemma 4.3, one knows that the balanced double star tree obtain the maximum exponential reduced second Zagreb index among double star trees. Also, by Lemma 4.1, Lemma 4.2 and Lemma 4.3, we can find the maximum exponential reduced second Zagreb index of a tree.

Theorem 4.1. *If $T \in \mathcal{T}_n$ $(n \geq 4)$ then*

$$e^{RM_2}(T) \leq e^{RM_2}\left(S_{\lfloor \frac{n-2}{2} \rfloor, \lceil \frac{n-2}{2} \rceil}\right),$$

where the equality holds if and only if $T \cong S_{\lfloor \frac{n-2}{2} \rfloor, \lceil \frac{n-2}{2} \rceil}$ and it holds that

$$e^{RM_2}\left(S_{\lfloor \frac{n-2}{2} \rfloor, \lceil \frac{n-2}{2} \rceil}\right) = \begin{cases} e^{\frac{1}{4}(n-2)^2} + n - 2, & \text{if} \quad n \equiv 0 \pmod 2, \\ e^{\frac{1}{4}(n-3)(n-1)} + n - 2, & \text{if} \quad n \equiv 1 \pmod 2. \end{cases}$$

5. Conclusion

In this study, we determine the minimum and maximum exponential reduced second Zagreb index of trees and chemical trees, and characterize the corresponding extremal (chemical) trees. A chemical tree is a tree of maximum degree at most four. Actually, a chemical tree models the skeleton of an acyclic molecule [25]. The results obtained in this paper may play a useful role in the QSAR and QSPR researches.

Recently, the study of the exponential topological indices caught some scholars' eyes. Cruz et al. [8,11] obtained extremal values of some exponential topological indices over trees and chemical trees. It is natural to study the extremal chemical trees for other exponential topological indices, such as the exponential general sum-connectivity index. On the other hand, one may also study the relationship between the exponential reduced second Zagreb index and some other topological indices such as the exponential ABC index, the exponential GA index and so on.

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