

Research Article

Exponential elliptic Sombor index of molecular trees

Wei Gao*

Department of Mathematics, Pennsylvania State University at Abington, Abington, PA 19001, USA

(Received: 22 November 2024. Received in revised form: 15 January 2025. Accepted: 20 January 2025. Published online: 22 January 2025.)

© 2025 the author. This is an open-access article under the CC BY (International 4.0) license (www.creativecommons.org/licenses/by/4.0/).

Abstract

Let G be a simple connected graph of order n with the vertex set $V(G)$ and edge set $E(G)$. For a vertex $v \in V(G)$, denote by $d_G(v)$ the degree of v in G . The exponential elliptic Sombor index of G is denoted by $e^{ESO}(G)$ and is defined as $e^{ESO}(G) = \sum_{v_i v_j \in E(G)} e^{(d_G(v_i) + d_G(v_j)) \sqrt{d_G^2(v_i) + d_G^2(v_j)}}$. In this paper, the minimum and maximum values of the exponential elliptic Sombor index of molecular trees of order n are obtained. Those molecular trees that achieve the obtained minimum and maximum values are also characterized.

Keywords: molecular tree; exponential elliptic Sombor index; extremal value.

2020 Mathematics Subject Classification: 05C09, 05C50, 05C92.

1. Introduction

All the graphs considered in this paper are simple and connected. Let G be such a graph with the vertex set $V(G)$ and edge set $E(G)$. For a vertex $v \in V(G)$, denote by $d_G(v)$ the degree of v in G . A tree is a connected acyclic graph. A molecular tree (or chemical tree) is a tree of maximum degree at most four.

From a geometric perspective, Gutman [2] introduced the Sombor index, which is defined as

$$SO(G) = \sum_{v_i v_j \in E(G)} \sqrt{d_G^2(v_i) + d_G^2(v_j)}.$$

The extremal properties of the Sombor index have been the subject of many publications, as demonstrated by the numerous results reported in [4].

In 2024, Gutman, Furtula, and Oz [3] introduced a new vertex-degree-based topological index, called the elliptic Sombor index, using a novel geometric method. The elliptic Sombor index of a graph G is defined as

$$ESO(G) = \sum_{v_i v_j \in E(G)} (d_G(v_i) + d_G(v_j)) \sqrt{d_G^2(v_i) + d_G^2(v_j)}. \quad (1)$$

In [3], several basic mathematical properties of this new index were established, and an extremal problem about this index for trees was studied. In [7], the maximum value of the elliptic Sombor index of trees with a given diameter or matching number or number of pendent vertices was determined. The extremal values of the elliptic Sombor index of unicyclic graphs were also found in [7]. Furthermore, those trees and unicyclic graphs that achieve the obtained extremal values were characterized in [7]. In [1], the extremal values of the elliptic Sombor index of chemical graphs and chemical trees with an equal number of vertices were determined. In [5], the bicyclic graph of a given order with the maximum elliptic Sombor index was determined. Furthermore, the ordering relations in benzenoid systems with respect to the elliptic Sombor index were given in [6].

The exponential elliptic Sombor index of a graph G is defined as follows:

$$e^{ESO}(G) = \sum_{v_i v_j \in E(G)} e^{(d_G(v_i) + d_G(v_j)) \sqrt{d_G^2(v_i) + d_G^2(v_j)}}. \quad (2)$$

In this paper, extremal values of the exponential elliptic Sombor index of molecular trees with a given order are determined. Those molecular trees that achieve the obtained extremal values are also characterized.

*E-mail address: wvg5121@psu.edu

2. Preliminaries

Let \mathcal{CT}_n be the set of all molecular trees of order n , and $T \in \mathcal{CT}_n$. A vertex v with $d_T(v) = i$ is called an i -degree vertex of T . An edge $e = uv$ with $d_T(u) = i$ and $d_T(v) = j$ is called an (i, j) -edge of T . The numbers of i -degree vertices and (i, j) -edges in T are denoted by $n_i = n_i(T)$ and $m_{ij} = m_{ij}(T)$, respectively. Then we have

$$\begin{cases} n_1 + n_2 + n_3 + n_4 = n, \\ n_1 + 2n_2 + 3n_3 + 4n_4 = 2(n - 1), \\ m_{12} + m_{13} + m_{14} = n_1, \\ m_{12} + 2m_{22} + m_{23} + m_{24} = 2n_2, \\ m_{13} + m_{23} + 2m_{33} + m_{34} = 3n_3, \\ m_{14} + m_{24} + m_{34} + 2m_{44} = 4n_4. \end{cases} \tag{3}$$

Let $f(x, y) = (x + y)\sqrt{x^2 + y^2}$. Then by (2), we have

$$\begin{aligned} e^{ESO}(T) &= \sum_{1 \leq i \leq j \leq 4} m_{ij} e^{f(i,j)} \\ &= e^{3\sqrt{5}}m_{12} + e^{4\sqrt{10}}m_{13} + e^{5\sqrt{17}}m_{14} + e^{8\sqrt{2}}m_{22} + e^{5\sqrt{13}}m_{23} + e^{12\sqrt{5}}m_{24} + e^{18\sqrt{2}}m_{33} + e^{35}m_{34} + e^{32\sqrt{2}}m_{44}. \end{aligned} \tag{4}$$

We now define three subsets $\mathcal{T}_0(n)$, $\mathcal{T}_1(n)$ and $\mathcal{T}_2(n)$ of \mathcal{CT}_n ($n \geq 5$) that will be used in Theorem 3.2.

- (1) $\mathcal{T}_0(n)$ consists of molecular trees on $n \equiv 0 \pmod{3}$ vertices with $m_{13} = m_{22} = m_{23} = m_{33} = m_{34} = 0$, $m_{12} = m_{24} = 1$, $m_{14} = \frac{2n-3}{3}$, and $m_{44} = \frac{n-6}{3}$.
- (2) $\mathcal{T}_1(n)$ consists of molecular trees on $n \equiv 1 \pmod{3}$ vertices with $m_{12} = m_{22} = m_{23} = m_{24} = m_{33} = 0$, $m_{13} = 2$, $m_{34} = 1$, $m_{14} = \frac{2n-5}{3}$, and $m_{44} = \frac{n-7}{3}$.
- (3) $\mathcal{T}_2(n)$ consists of molecular trees on $n \equiv 2 \pmod{3}$ vertices with $m_{12} = m_{13} = m_{22} = m_{23} = m_{24} = m_{33} = m_{34} = 0$, $m_{14} = \frac{2n+2}{3}$, and $m_{44} = \frac{n-5}{3}$.

For each of the three subsets of \mathcal{CT}_n defined above, a molecular tree is shown in Figure 2.1. This means that all of these subsets are nonempty.

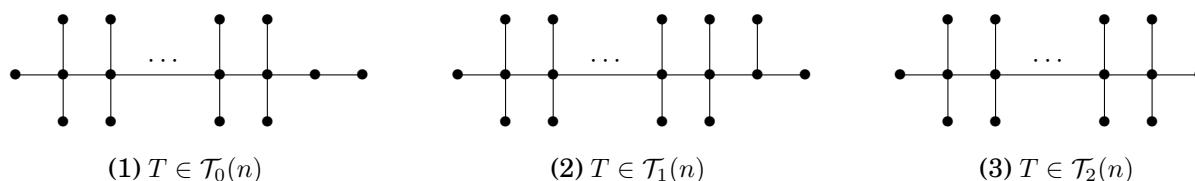


Figure 2.1: Some examples of molecular trees.

3. Molecular trees with the extremal exponential elliptic Sombor indices

In this section, we give the minimum and maximum values of the exponential elliptic Sombor indices over \mathcal{CT}_n , and characterize those molecular trees that achieve the minimum and maximum values, respectively.

Theorem 3.1. Let $T \in \mathcal{CT}_n$ with $n \geq 3$. Then

$$e^{ESO}(T) \geq e^{8\sqrt{2}}n - 3e^{8\sqrt{2}} + 2e^{3\sqrt{5}}, \tag{5}$$

where the equality holds if and only if T is a path of order n .

Proof. Let $T \in \mathcal{CT}_n$. Solving the system (3) with unknowns $m_{12}, m_{22}, n_1, n_2, n_3, n_4$, we obtain

$$\left\{ \begin{array}{l} m_{12} = -\frac{2m_{13}}{3} - \frac{m_{14}}{2} + \frac{m_{23}}{3} + \frac{m_{24}}{2} + \frac{2m_{33}}{3} + \frac{5m_{34}}{6} + m_{44} + 2, \\ m_{22} = -\frac{m_{13}}{3} - \frac{m_{14}}{2} - \frac{4m_{23}}{3} - \frac{3m_{24}}{2} - \frac{5m_{33}}{3} - \frac{11m_{34}}{6} - 2m_{44} + n - 3, \\ n_1 = \frac{m_{13}}{3} + \frac{m_{14}}{2} + \frac{m_{23}}{3} + \frac{m_{24}}{2} + \frac{2m_{33}}{3} + \frac{5m_{34}}{6} + m_{44} + 2, \\ n_2 = -\frac{2m_{13}}{3} - \frac{3m_{14}}{4} - \frac{2m_{23}}{3} - \frac{3m_{24}}{4} - \frac{4m_{33}}{3} - \frac{17m_{34}}{12} - \frac{3m_{44}}{2} + n - 2, \\ n_3 = \frac{1}{3}(m_{13} + m_{23} + 2m_{33} + m_{34}), \\ n_4 = \frac{1}{4}(m_{14} + m_{24} + m_{34} + 2m_{44}). \end{array} \right. \tag{6}$$

Replacing the values of m_{12} and m_{22} in (4), and then after simplification, we have

$$e^{ESO}(T) = A_0 + A_{13}m_{13} + A_{14}m_{14} + A_{23}m_{23} + A_{24}m_{24} + A_{33}m_{33} + A_{34}m_{34} + A_{44}m_{44}, \tag{7}$$

where

$$\left\{ \begin{array}{l} A_0 = e^{8\sqrt{2}}n - 3e^{8\sqrt{2}} + 2e^{3\sqrt{5}}, \\ A_{13} = -\frac{1}{3}e^{8\sqrt{2}} - \frac{2e^{3\sqrt{5}}}{3} + e^{4\sqrt{10}} \approx 283628.0, \\ A_{14} = -\frac{1}{2}e^{8\sqrt{2}} - \frac{e^{3\sqrt{5}}}{2} + e^{5\sqrt{17}} \approx 8.97822 \times 10^8, \\ A_{23} = -\frac{4}{3}e^{8\sqrt{2}} + \frac{e^{3\sqrt{5}}}{3} + e^{5\sqrt{13}} \approx 6.7399 \times 10^7, \\ A_{24} = -\frac{3}{2}e^{8\sqrt{2}} + \frac{e^{3\sqrt{5}}}{2} + e^{12\sqrt{5}} \approx 4.50136 \times 10^{11}, \\ A_{33} = -\frac{5}{3}e^{8\sqrt{2}} + e^{18\sqrt{2}} + \frac{2e^{3\sqrt{5}}}{3} \approx 1.13588 \times 10^{11}, \\ A_{34} = e^{35} - \frac{11e^{8\sqrt{2}}}{6} + \frac{5e^{3\sqrt{5}}}{6} \approx 1.58601 \times 10^{15}, \\ A_{44} = -2e^{8\sqrt{2}} + e^{32\sqrt{2}} + e^{3\sqrt{5}} \approx 4.50739 \times 10^{19}. \end{array} \right. \tag{8}$$

Since all $A_{13}, A_{14}, A_{23}, A_{24}, A_{33}, A_{34}, A_{44}$ are positive, Equation (7) gives

$$e^{ESO}(T) \geq A_0,$$

where the equality holds if and only if

$$m_{13} = m_{14} = m_{23} = m_{24} = m_{33} = m_{34} = m_{44} = 0,$$

that is, T is a path of order n . □

Theorem 3.2. Let $T \in \mathcal{CT}_n$ with $n \geq 5$. Then

$$e^{ESO}(T) \leq \begin{cases} \frac{1}{3} \left(e^{32\sqrt{2}} + 2e^{5\sqrt{17}} \right) n - 2e^{32\sqrt{2}} + e^{3\sqrt{5}} + e^{12\sqrt{5}} - e^{5\sqrt{17}}, & \text{if } n \equiv 0 \pmod{3}, \\ \frac{1}{3} \left(e^{32\sqrt{2}} + 2e^{5\sqrt{17}} \right) n + 2e^{4\sqrt{10}} + e^{35} - \frac{7e^{32\sqrt{2}}}{3} - \frac{5e^{5\sqrt{17}}}{3}, & \text{if } n \equiv 1 \pmod{3}, \\ \frac{1}{3} \left(e^{32\sqrt{2}} + 2e^{5\sqrt{17}} \right) n - \frac{5e^{32\sqrt{2}}}{3} + \frac{2e^{5\sqrt{17}}}{3}, & \text{if } n \equiv 2 \pmod{3}, \end{cases} \tag{9}$$

where the equality holds if and only if $T \in \mathcal{T}_i(n)$ for $n \equiv i \pmod{3}$ ($i = 0, 1, 2$).

Proof. Let $T \in \mathcal{CT}_n$. Solving the system (3) with unknowns $m_{12}, m_{24}, n_1, n_2, n_3, n_4$, we obtain

$$\begin{cases} m_{12} = \frac{n+3}{3} - \frac{7m_{13}}{9} - \frac{2m_{14}}{3} - \frac{m_{22}}{3} - \frac{m_{23}}{9} + \frac{m_{33}}{9} + \frac{2m_{34}}{9} + \frac{m_{44}}{3}, \\ m_{24} = \frac{2n-6}{3} - \frac{2m_{13}}{9} - \frac{m_{14}}{3} - \frac{2m_{22}}{3} - \frac{8m_{23}}{9} - \frac{10m_{33}}{9} - \frac{11m_{34}}{9} - \frac{4m_{44}}{3}, \\ n_1 = \frac{n+3}{3} + \frac{2m_{13}}{9} + \frac{m_{14}}{3} - \frac{m_{22}}{3} - \frac{m_{23}}{9} + \frac{m_{33}}{9} + \frac{2m_{34}}{9} + \frac{m_{44}}{3}, \\ n_2 = \frac{n-2}{2} - \frac{m_{13}}{2} - \frac{m_{14}}{2} + \frac{m_{22}}{2} - \frac{m_{33}}{2} - \frac{m_{34}}{2} - \frac{m_{44}}{2}, \\ n_3 = \frac{1}{3}(m_{13} + m_{23} + 2m_{33} + m_{34}), \\ n_4 = \frac{n-3}{6} - \frac{m_{13}}{18} + \frac{m_{14}}{6} - \frac{m_{22}}{6} - \frac{2m_{23}}{9} - \frac{5m_{33}}{18} - \frac{m_{34}}{18} + \frac{m_{44}}{6}. \end{cases} \tag{10}$$

Replacing the values of m_{12} and m_{24} in (4), then after simplification, we have

$$e^{ESO}(T) = B_0 + B_{13}m_{13} + B_{14}m_{14} + B_{22}m_{22} + B_{23}m_{23} + B_{33}m_{33} + B_{34}m_{34} + B_{44}m_{44}, \tag{11}$$

where

$$\begin{cases} B_0 = \frac{1}{3} (e^{3\sqrt{5}} + 2e^{12\sqrt{5}}) n + e^{3\sqrt{5}} - 2e^{12\sqrt{5}}, \\ B_{13} = -\frac{7}{9}e^{3\sqrt{5}} - \frac{2e^{12\sqrt{5}}}{9} + e^{4\sqrt{10}} \approx -1.0003 \times 10^{11}, \\ B_{14} = -\frac{2}{3}e^{3\sqrt{5}} - \frac{e^{12\sqrt{5}}}{3} + e^{5\sqrt{17}} \approx -1.49147 \times 10^{11}, \\ B_{22} = e^{8\sqrt{2}} - \frac{e^{3\sqrt{5}}}{3} - \frac{2e^{12\sqrt{5}}}{3} \approx -3.00091 \times 10^{11}, \\ B_{23} = -\frac{1}{9}e^{3\sqrt{5}} - \frac{8e^{12\sqrt{5}}}{9} + e^{5\sqrt{13}} \approx -4.00053 \times 10^{11}, \\ B_{33} = e^{18\sqrt{2}} + \frac{e^{3\sqrt{5}}}{9} - \frac{10e^{12\sqrt{5}}}{9} \approx -3.86563 \times 10^{11}, \\ B_{34} = e^{35} + \frac{2e^{3\sqrt{5}}}{9} - \frac{11e^{12\sqrt{5}}}{9} \approx 1.58546 \times 10^{15}, \\ B_{44} = e^{32\sqrt{2}} + \frac{e^{3\sqrt{5}}}{3} - \frac{4e^{12\sqrt{5}}}{3} \approx 4.50739 \times 10^{19}. \end{cases} \tag{12}$$

In order to find the maximum value of $e^{ESO}(T)$, we consider the following four cases.

Case 1. $n_3 = 0$.

In this case, we have $m_{13} = m_{23} = m_{33} = m_{34} = 0$. By (11), we have

$$e^{ESO}(T) = B_0 + B_{14}m_{14} + B_{22}m_{22} + B_{44}m_{44}. \tag{13}$$

Subcase 1.1. $n_2 = 0$.

Note that $m_{12} = m_{22} = m_{24} = 0$. By (3), we have $n_4 = \frac{n-2}{3}$, $n_1 = \frac{2n+2}{3}$, $m_{14} = \frac{2n+2}{3}$, and $m_{44} = \frac{n-5}{3}$. So $n \equiv 2 \pmod{3}$ and $T \in \mathcal{T}_2(n)$. Thus, by (13), we have

$$e^{ESO}(T) = B_0 + \frac{2n+2}{3}B_{14} + \frac{n-5}{3}B_{44}. \tag{14}$$

Subcase 1.2. $n_2 = 1$.

Note that $m_{22} = 0$, $m_{12} \leq 1$, and $m_{12} + m_{24} = 2$. By the first two equations in (3), we have $n_4 = \frac{n-3}{3}$ and $n_1 = \frac{2n}{3}$. So, $n \equiv 0 \pmod{3}$.

If $m_{12} = 1$, then $m_{24} = 1$. By the third and sixth equations in (3), we have $m_{14} = \frac{2n-3}{3}$ and $m_{44} = \frac{n-6}{3}$. By (13), we have

$$e^{ESO}(T) = B_0 + \frac{2n-3}{3}B_{14} + \frac{n-6}{3}B_{44}.$$

If $m_{12} = 0$, then $m_{24} = 2$. By the third and sixth equations in (3), we have $m_{14} = \frac{2n}{3}$ and $m_{44} = \frac{n-9}{3}$. By (13), we have

$$e^{ESO}(T) = B_0 + \frac{2n}{3}B_{14} + \frac{n-9}{3}B_{44}.$$

Note that

$$\frac{2n-3}{3}B_{14} + \frac{n-6}{3}B_{44} > \frac{2n}{3}B_{14} + \frac{n-9}{3}B_{44}.$$

Thus, for the considered subcase, we have

$$e^{ESO}(T) \leq B_0 + \frac{2n-3}{3}B_{14} + \frac{n-6}{3}B_{44}, \tag{15}$$

where the equality is true if and only if $m_{12} = m_{24} = 1$, $m_{14} = \frac{2n-3}{3}$, and $m_{44} = \frac{n-6}{3}$, that is, $T \in \mathcal{T}_0(n)$.

Subcase 1.3. $n_2 \geq 2$.

By the first two equations in (3), we have that $3n_1 + 2n_2 = 2n + 2$ and $n_2 + 3n_4 = n - 2$. Then,

$$n_1 = \frac{2n - 2n_2 + 2}{3} \quad \text{and} \quad n_4 = \frac{n - n_2 - 2}{3}.$$

Note that $m_{12} \leq n_2$, $m_{44} \leq n_4 - 1$, and $m_{12} + m_{14} = n_1$. Hence,

$$m_{14} = n_1 - m_{12} \geq n_1 - n_2 = \frac{2n - 5n_2 + 2}{3}$$

and

$$m_{44} \leq n_4 - 1 = \frac{n - n_2 - 5}{3}.$$

By (12) and (13), we have

$$\begin{aligned} e^{ESO}(T) &\leq B_0 + \frac{2n - 5n_2 + 2}{3}B_{14} + \frac{n - n_2 - 5}{3}B_{44} \\ &= B_0 + \frac{2n + 2}{3}B_{14} + \frac{n - 5}{3}B_{44} - \left(\frac{5}{3}B_{14} + \frac{1}{3}B_{44}\right)n_2. \end{aligned}$$

Note that

$$\frac{5}{3}B_{14} + \frac{1}{3}B_{44} \approx 1.50246 \times 10^{19} > 0.$$

So,

$$\begin{aligned} e^{ESO}(T) &\leq B_0 + \frac{2n + 2}{3}B_{14} + \frac{n - 5}{3}B_{44} - 2\left(\frac{5}{3}B_{14} + \frac{1}{3}B_{44}\right) \\ &= B_0 + \frac{2n - 8}{3}B_{14} + \frac{n - 7}{3}B_{44}. \end{aligned} \tag{16}$$

Case 2. $n_3 = 1$ and $n_2 = 0$.

Observe that $m_{12} = m_{22} = m_{23} = m_{24} = m_{33} = 0$, and $m_{13} + m_{34} = 3$. By (11), we have

$$e^{ESO}(T) = B_0 + B_{13}m_{13} + B_{14}m_{14} + B_{34}m_{34} + B_{44}m_{44}. \tag{17}$$

By the first two equations in (3), we have $n_4 = \frac{n-4}{3}$ and $n_1 = \frac{2n+1}{3}$. So, $n \equiv 1 \pmod{3}$. Note that $m_{13} \leq 2$. Table 3.1 gives the values of m_{14} and m_{44} for all possible choices of (m_{13}, m_{34}) by the third and sixth equations in (3).

Table 3.1 The values of m_{14} and m_{44} for all possible choices of (m_{13}, m_{34}) .

m_{13}	m_{34}	m_{14}	m_{44}
2	1	$\frac{2n-5}{3}$	$\frac{n-7}{3}$
1	2	$\frac{2n-2}{3}$	$\frac{n-10}{3}$
0	3	$\frac{2n+1}{3}$	$\frac{n-13}{3}$

By (17), Table 3.1, and a direct calculation, we have

$$e^{ESO}(T) \leq B_0 + 2B_{13} + \frac{2n-5}{3}B_{14} + B_{34} + \frac{n-7}{3}B_{44}, \tag{18}$$

where the equality is true if and only if $m_{13} = 2, m_{34} = 1, m_{14} = \frac{2n-5}{3}$, and $m_{44} = \frac{n-7}{3}$, that is, $T \in \mathcal{T}_1(n)$.

Case 3. $n_3 = 1$ and $n_2 \geq 1$.

By the first three equations in (3), we have that $3n_1 + 2n_2 = 2n + 1, n_2 + 3n_4 = n - 4$, and $m_{12} + m_{13} + m_{14} = n_1$. Note that $m_{12} \leq n_2$. Then,

$$n_1 = \frac{2n - 2n_2 + 1}{3}, \quad n_4 = \frac{n - n_2 - 4}{3}, \quad \text{and} \quad m_{14} = n_1 - m_{12} - m_{13} \geq n_1 - n_2 - m_{13} = \frac{2n - 5n_2 + 1}{3} - m_{13}.$$

Note also that

$$m_{33} = 0, \quad m_{13} \leq 2, \quad m_{34} \leq 3, \quad m_{44} \leq n_4 - 1 = \frac{n - n_2 - 7}{3}, \quad \text{and} \quad B_{13} > B_{14}.$$

Thus, by (11) and (12), we have

$$\begin{aligned} e^{ESO}(T) &\leq B_0 + B_{13}m_{13} + B_{14}m_{14} + B_{34}m_{34} + B_{44}m_{44} \\ &\leq B_0 + B_{13}m_{13} + \left(\frac{2n - 5n_2 + 1}{3} - m_{13}\right)B_{14} + 3B_{34} + \frac{n - n_2 - 7}{3}B_{44} \\ &= B_0 + (B_{13} - B_{14})m_{13} + \frac{2n - 5n_2 + 1}{3}B_{14} + 3B_{34} + \frac{n - n_2 - 7}{3}B_{44} \\ &\leq B_0 + 2(B_{13} - B_{14}) + \frac{2n - 5n_2 + 1}{3}B_{14} + 3B_{34} + \frac{n - n_2 - 7}{3}B_{44} \\ &= B_0 + 2B_{13} + \frac{2n - 5}{3}B_{14} + 3B_{34} + \frac{n - 7}{3}B_{44} - \left(\frac{5}{3}B_{14} + \frac{1}{3}B_{44}\right)n_2. \end{aligned}$$

Since

$$\frac{5}{3}B_{14} + \frac{1}{3}B_{44} \approx 1.50246 \times 10^{19} > 0,$$

we have

$$\begin{aligned} e^{ESO}(T) &\leq B_0 + 2B_{13} + \frac{2n-5}{3}B_{14} + 3B_{34} + \frac{n-7}{3}B_{44} - \left(\frac{5}{3}B_{14} + \frac{1}{3}B_{44}\right)n_2 \\ &= B_0 + 2B_{13} + \frac{2n-10}{3}B_{14} + 3B_{34} + \frac{n-8}{3}B_{44}. \end{aligned} \tag{19}$$

Case 4. $n_3 \geq 2$.

By the first three equations in (3), we have that $3n_1 + 2n_2 + n_3 = 2n + 2, n_2 + 2n_3 + 3n_4 = n - 2$, and $m_{12} + m_{13} + m_{14} = n_1$. Note that $m_{12} \leq n_2$. Then

$$n_1 = \frac{2n + 2 - 2n_2 - n_3}{3}, \quad n_4 = \frac{n - 2 - n_2 - 2n_3}{3}, \quad \text{and} \quad m_{14} = n_1 - m_{12} - m_{13} \geq n_1 - n_2 - m_{13} = \frac{2n + 2 - 5n_2 - n_3}{3} - m_{13}.$$

Observe also that

$$m_{44} \leq n_4 - 1 = \frac{n - 5 - n_2 - 2n_3}{3} \quad \text{and} \quad m_{34} \leq 3n_3 - m_{13}.$$

Thus, by (11) and (12), we have

$$\begin{aligned} e^{ESO}(T) &\leq B_0 + B_{13}m_{13} + B_{14}m_{14} + B_{34}m_{34} + B_{44}m_{44} \\ &\leq B_0 + B_{13}m_{13} + \left(\frac{2n + 2 - 5n_2 - n_3}{3} - m_{13}\right)B_{14} + (3n_3 - m_{13})B_{34} + \frac{n - 5 - n_2 - 2n_3}{3}B_{44} \\ &= B_0 + \frac{2n + 2}{3}B_{14} + \frac{n - 5}{3}B_{44} + (B_{13} - B_{14} - B_{34})m_{13} - \left(\frac{5}{3}B_{14} + \frac{1}{3}B_{44}\right)n_2 - \left(\frac{1}{3}B_{14} - 3B_{34} + \frac{2}{3}B_{44}\right)n_3. \end{aligned}$$

Note that

$$B_{13} - B_{14} - B_{34} \approx -1.58541 \times 10^{15} < 0,$$

$$\frac{5}{3}B_{14} + \frac{1}{3}B_{44} \approx 1.50246 \times 10^{19} > 0, \quad \text{and}$$

$$\frac{1}{3}B_{14} - 3B_{34} + \frac{2}{3}B_{44} \approx 3.00445 \times 10^{19} > 0.$$

Hence,

$$\begin{aligned} e^{ESO}(T) &\leq B_0 + \frac{2n+2}{3}B_{14} + \frac{n-5}{3}B_{44} - 2\left(\frac{1}{3}B_{14} - 3B_{34} + \frac{2}{3}B_{44}\right) \\ &= B_0 + \frac{2n}{3}B_{14} + 6B_{34} + \frac{n-9}{3}B_{44}. \end{aligned} \quad (20)$$

Combining the discussions of Cases 1–4, and noting that

$$\begin{aligned} \frac{2n-8}{3}B_{14} + \frac{n-7}{3}B_{44} &> 2B_{13} + \frac{2n-10}{3}B_{14} + 3B_{34} + \frac{n-8}{3}B_{44} > \frac{2n}{3}B_{14} + 6B_{34} + \frac{n-9}{3}B_{44}, \\ \frac{2n-3}{3}B_{14} + \frac{n-6}{3}B_{44} &> \frac{2n-8}{3}B_{14} + \frac{n-7}{3}B_{44}, \\ 2B_{13} + \frac{2n-5}{3}B_{14} + B_{34} + \frac{n-7}{3}B_{44} &> \frac{2n-8}{3}B_{14} + \frac{n-7}{3}B_{44}, \\ \frac{2n+2}{3}B_{14} + \frac{n-5}{3}B_{44} &> \frac{2n-8}{3}B_{14} + \frac{n-7}{3}B_{44}, \end{aligned}$$

we arrive at the following conclusions:

- If $n \equiv 0 \pmod{3}$, then by (15), (16), (19), and (20), T has the maximum exponential elliptic Sombor index over \mathcal{CT}_n if and only if $T \in \mathcal{T}_0(n)$, and this maximum value is given in (15);
- If $n \equiv 1 \pmod{3}$, then by (16), (18), (19), and (20), T has the maximum exponential elliptic Sombor index over \mathcal{CT}_n if and only if $T \in \mathcal{T}_1(n)$, and this maximum value is given in (18);
- If $n \equiv 2 \pmod{3}$, then by (14), (16), (19), and (20), T has the maximum exponential elliptic Sombor index over \mathcal{CT}_n if and only if $T \in \mathcal{T}_2(n)$, and this maximum value is given in (14).

This completes the proof of Theorem 3.2. □

Acknowledgment

The author would like to thank the anonymous reviewers for their valuable comments and suggestions.

References

- [1] C. Espinal, I. Gutman, J. Rada, Elliptic Sombor index of chemical graphs, *Commun. Comb. Optim.*, In press, DOI:10.22049/cc.2024.29404.1977.
- [2] I. Gutman, Geometric approach to degree-based topological indices: Sombor indices, *MATCH Commun. Math. Comput. Chem.* **86** (2021) 11–16.
- [3] I. Gutman, B. Furtula, M. S. Oz, Geometric approach to vertex-degree-based topological indices-elliptic Sombor index, theory and application, *Int. J. Quantum Chem.* **124** (2024) #e27346.
- [4] H. Liu, I. Gutman, L. You, Y. Huang, Sombor index: review of extremal results and bounds, *J. Math. Chem.* **60** (2022) 771–798.
- [5] F. Qi, Z. Lin, Maximal elliptic Sombor index of bicyclic graphs, *Contrib. Math.* **10** (2024) 25–29.
- [6] J. Rada, J. M. Rodríguez, J. M. Sigarreta, Sombor index and elliptic Sombor index of benzenoid systems, *Appl. Math. Comput.* **475** (2024) #128756.
- [7] Z. Tang, Y. Li, H. Deng, Elliptic Sombor index of trees and unicyclic graphs, *Electron. J. Math.* **7** (2024) 19–34.