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On the Ordering of Chemical Graphs by Elliptic Sombor Index

Fateme Movahedi[a,*], **Mohammad Hadi Akhbari**[b]

[a] *Department of Mathematics, Faculty of Sciences, Golestan University, Gorgan, Iran*

[b] *Department of Mathematics, Es.C., Islamic Azad University, Estahban, Iran*

f.movahedi@gu.ac.ir, hadi.akhbari@iau.ac.ir

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Abstract

The elliptic Sombor index of a graph G with the edge set $E(G)$ is a recently introduced degree-based topological index defined as

$$ESO(G) = \sum_{uv \in E(G)} (d(u) + d(v)) \sqrt{d(u)^2 + d(v)^2},$$

where d_u denotes the degree of vertex u.

In this paper, we present the ordering of the minimum elliptic Sombor index among all chemical trees, as well as chemical unicyclic, bicyclic, and tricyclic graphs.

1 Introduction

Let G be a graph with a vertex set $V(G)$ and an edge set $E(G)$. For any vertex $u \in V(G)$, its degree, denoted by $d_G(u)$ or simply d_u, is the number of edges incident to it. The set of all vertices adjacent to u is represented

*Corresponding author.

by $N_G(u)$. A vertex of degree one is called a pendent vertex. The symbols $\Delta = \Delta(G)$ and $n_i = n_i(G)$ denote the maximum degree and the number of vertices of degree i in G, respectively. Note that the total number of vertices is $|V(G)| = \sum_{i=1}^{\Delta} n_i$. The number of edges connecting a vertex of degree i to a vertex of degree j is denoted by m_{ij}. The degree sequence of a graph G is the sequence of its vertex degrees arranged in non-increasing order, $\mathcal{D}(G) = (d_1, d_2, \ldots, d_n)$ in which d_i is the degree of the vertex v_i. For any terminology and notation not defined in this paper, we refer the reader to standard texts such as [8].

For any edge $e \in E(G)$, the graph $G - \{e\}$ is formed by removing e from $E(G)$ while retaining the original vertex set $V(G)$. The removal of multiple edges, such as $e_1, \ldots, e_k$, is defined as a sequential process, where $G - \{e_1, \ldots, e_k\}$ is equivalent to $(G - \{e_1, \ldots, e_{k-1}\}) - \{e_k\}$.

A chemical graph provides a mathematical model of a molecule, where vertices represent atoms with a maximum degree of at most four, and edges correspond to the chemical bonds connecting them. From this structure, a topological index can be calculated, which is a numerical value that quantifies the molecular topology and is invariant under graph isomorphism [9]. These descriptors are foundational in quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) investigations. They facilitate the prediction of various physicochemical properties, such as boiling point, stability, and reactivity, by establishing a mathematical correlation between a molecule's structure and its behavior [6]. The ability to forecast these properties without physical synthesis makes topological indices invaluable for virtual screening in drug discovery and materials science. Over the past few years, a variety of novel degree-based indices have been proposed to enhance the predictive power of these models. Among the most significant recent contributions are the Sombor index [10], the Diminished Sombor index [17], and the Euler Sombor index [25]. For a more detailed exploration of the mathematical properties of topological indices and their applications, readers are encouraged to consult comprehensive surveys and key papers in the field [1,2,13,16,18,19,26].

The recently introduced elliptic Sombor index by Gutman in 2024 [11] represents a novel approach to quantifying molecular structure within the framework of topological indices, building upon the established utility of the Sombor index in correlating structure with physicochemical properties. The elliptic Sombor index is defined as follows

$$ESO(G) = \sum_{uv \in E(G)} (d(u) + d(v)) \sqrt{d(u)^2 + d(v)^2}.$$

Recent scholarship has extensively explored the mathematical properties and chemical applications of the elliptic Sombor (ESO) index. Theoretical foundations and optimization problems for the general ESO index have been established by Gutman et al. [11] and Rada et al. [23], while Kulli [15] expanded the framework by introducing a modified version. Significant research has focused on determining extremal values and characterizing specific graph structures, including chemical graphs and trees [5], benzenoid systems [24], bicyclic graphs [22], and polymer-like networks constructed from primary subgraphs [7]. Ahmad, Das and Farooq further analyzed structural properties of the elliptic Sombor index and illustrated its usefulness through several chemical applications [3], whereas Ahmad and Gutman derived sharp degree-based bounds for the ESO index of molecular trees with prescribed order and maximum degree [4]. Movahedi obtained additional general results on the elliptic Sombor index and provided detailed relations between this index and various classical degree-based topological indices, such as the Zagreb, Forgotten, Randić and Sombor indices [20,21]. In the context of chemical modeling, Kirana et al. [14] evaluated the predictive potential of the ESO index for polycyclic aromatic hydrocarbons using regression analysis.

In this paper, we systematically characterize the extremal structures for the elliptic Sombor index within specific classes of chemical graphs. By applying graph transformations that strictly decrease the index value, we determine the ordering of the minimum elliptic Sombor index for chemical trees, chemical unicyclic graphs, chemical bicyclic graphs, and chemical tricyclic graphs. These results contribute to the broader understanding of how structural variations in chemical networks influence their degree-based topological properties.

2 Preliminaries

In this section, we introduce several graph operations that are shown to decrease the value of the elliptic Sombor index. These operations are then applied to characterize the extremal graphs for this index within the classes of chemical graphs including unicyclic graphs, bicyclic graphs, tricyclic graphs, and chemical trees.

Operation 1. Let G_0 be a connected graph with a vertex w such that $d_{G_0}(w) = 1, 2$ or 3 and $P_1 = x_1 \cdots x_t$ and $P_2 = y_1 \cdots y_s$ be two paths of order t and s, respectively. Let G be the graph obtained from G_0 by attaching edges wx_1 and wy_1. Define $G^* = G - \{wx_1\} + \{x_1y_s\}$.

Lemma 1. *Let G and G^* be graphs described in Operation 1. Then*

$$ESO(G^*) < ESO(G).$$

Proof. Suppose that $d_{G_0}(w) = r = 1, 2$ or 3 and $N_{G_0}(w) = \{w_1, \ldots, w_r\}$ where $d_{G_0}(w_i) = d_i$ for $1 \leq i \leq r$. Let $\Theta = ESO(G^*) - ESO(G)$. We consider the following cases.
Case 1. Let $s = t = 1$. Therefore, we get

$$\begin{aligned}
\Theta =& \left[3\sqrt{5} + (r+3)\sqrt{(r+1)^2+4} + \sum_{i=1}^{r}(r+1+d_i)\sqrt{(r+1)^2+d_i^2}\right] \\
&- \left[2(r+3)\sqrt{(r+2)^2+1} + \sum_{i=1}^{r}(r+2+d_i)\sqrt{(r+2)^2+d_i^2}\right] \\
&= 3\sqrt{5} + (r+3)\left[\sqrt{(r+1)^2+4} - 2\sqrt{(r+2)^2+1}\right] \\
&+ \sum_{i=1}^{r}\left[(r+1+d_i)\sqrt{(r+1)^2+d_i^2} - (r+2+d_i)\sqrt{(r+2)^2+d_i^2}\right] \\
&< 0,
\end{aligned}$$

for $r = 1, 2$ or 3.
Case 2. Let $s = 1$ and $t \geq 2$ or $s \geq 2$ and $t = 1$. Without loss of generality, we consider $t = 1$ and $s \geq 2$. Therefore,

$$\Theta = \left[4\sqrt{8} + (r+3)\sqrt{(r+1)^2+4} + \sum_{i=1}^{r}(r+1+d_i)\sqrt{(r+1)^2+d_i^2}\right]$$

$$
\begin{aligned}
&- \Big[(r+3)\sqrt{(r+2)^2+1} + (r+4)\sqrt{(r+2)^2+4} \\
&+ \sum_{i=1}^{r}(r+2+d_i)\sqrt{(r+2)^2+d_i^2}\Big] \\
&= 8\sqrt{2} + (r+3)\left[\sqrt{(r+1)^2+4} - \sqrt{(r+2)^2+1}\right] \\
&- (r+4)\sqrt{(r+2)^2+4} \\
&+ \sum_{i=1}^{r}\left[(r+1+d_i)\sqrt{(r+1)^2+d_i^2} - (r+2+d_i)\sqrt{(r+2)^2+d_i^2}\right] \\
&< 0.
\end{aligned}
$$

Since $r = 1, 2$ or 3, we have $ESO(G^*) < ESO(G)$.
Case 3. Let $s, t \geq 2$. Then, we get

$$
\begin{aligned}
ESO(G^*) - ESO(G) = &\Big[8\sqrt{2} + (r+3)\sqrt{(r+1)^2+4} \\
&+ \sum_{i=1}^{r}(r+1+d_i)\sqrt{(r+1)^2+d_i^2}\Big] \\
&- \Big[3\sqrt{5} + 2(r+4)\sqrt{(r+2)^2+4} \\
&+ \sum_{i=1}^{r}(r+2+d_i)\sqrt{(r+2)^2+d_i^2}\Big] \\
&< \left[8\sqrt{2} + (r+3)\sqrt{(r+1)^2+4}\right] \\
&- \left[3\sqrt{5} + 2(r+4)\sqrt{(r+2)^2+4}\right].
\end{aligned}
$$

For $r = 1$, we have $ESO(G^*) - ESO(G) < 16\sqrt{2} - 10\sqrt{13} - 3\sqrt{5} < 0$, for $r = 2$, we have $ESO(G^*) - ESO(G) < 5\sqrt{13} + 8\sqrt{2} - 27\sqrt{5} < 0$, and for $r = 3$, we have $ESO(G^*) - ESO(G) < 6\sqrt{20} + 8\sqrt{2} - 14\sqrt{29} - 3\sqrt{5} < 0$. This completes the proof. ■

Operation 2. Let G_0 be a connected graph with vertices $w_i \in V(G_0)$, $1 \leq i \leq 4$, where $d_{G_0}(w_1) = d_{G_0}(w_4) = 1$, $d_{G_0}(w_3) \geq 2$ and $d_{G_0}(w_2) = 3$ or 4. Let $P_1 = x_1 \cdots x_t$ and $P_2 = y_1 \cdots y_s$ be two paths of order t and s, respectively. Let G be the graph obtained from G_0, P_1 and P_2 by attaching edges w_1x_1 and w_4y_1. Define $G^* = G - \{w_1x_1\} + \{y_sx_1\}$.

Lemma 2. *Let G and G^* be graphs described in Operation 2. Then*

$$ESO(G^*) < ESO(G).$$

Proof. Suppose that $d_{G_0}(w_2) = r$. Thus

$$\begin{aligned} ESO(G^*) - ESO(G) &= \left[8\sqrt{2} + (r+1)\sqrt{r^2+1}\right] \\ &\quad - \left[3\sqrt{5} + (r+4)\sqrt{(r+2)^2+4}\right] \\ &< 0, \end{aligned}$$

for $r = 3$ or 4. This completes the proof. ■

Operation 3. Let G_0 be a connected graph with vertices w and w' where $d_{G_0}(w) = 2$ or 3 and $d_{G_0}(w') = 2$ or 3. Let $P_1 = x_1 \cdots x_t$ and $P_2 = y_1 \cdots y_s$ be two paths of order t and s, respectively. Let G be the graph obtained from G_0, P_1 and P_2 by attaching edges wx_1 and $w'y_1$. Define $G^* = G - \{wx_1\} + \{x_1y_s\}$.

Lemma 3. *Let G and G^* be graphs described in Operation 3. Then*

$$ESO(G^*) < ESO(G).$$

Proof. Suppose that $d_{G_0}(w) = r$ and $N_{G_0}(w) = \{w_1, \ldots, w_r\}$ where $d_{G_0}(w_i) = d_i$ for $1 \le i \le r$. Therefore, we get

$$\begin{aligned} ESO(G^*) - ESO(G) &= \left[16\sqrt{2} + \sum_{i=1}^{r}(r+d_i)\sqrt{r^2+d_i^2}\right] \\ &\quad - 3\sqrt{5} + (r+3)\sqrt{(r+1)^2+4} \\ &\quad - \sum_{i=1}^{r}(r+1+d_i)\sqrt{(r+1)^2+d_i^2} \\ &< 16\sqrt{2} - 3\sqrt{5} - (r+3)\sqrt{(r+1)^2+4} < 0, \end{aligned}$$

for $r = 2$ or 3. For the remaining cases, the results hold by simple calculations. ■

Operation 4. Let G_i be connected graphs with vertices $w_i \in V(G_i)$ where $d_{G_i}(w_i) = 2$ for $i = 1, 2, 3$. Let $P_1 = x_1 \cdots x_t$ and $P_2 = y_1 \cdots y_s$ be two paths of order t and s, respectively. Let G be the graph obtained from G_i for $i = 1, 2, 3$, P_1 and P_2 by attaching edges w_1x_1, w_1w_2, w_2w_3, and w_3y_1. Define $G^* = G - \{x_1x_2, w_1w_2, w_2w_3, y_1y_2\} + \{x_2w_1, x_tw_2, w_2y_t, y_sw_3\}$.

Lemma 4. *Let G and G^* be graphs described in Operation 4. Then*

$$ESO(G^*) < ESO(G).$$

Proof. We have

$$ESO(G^*) - ESO(G) = \left(8\sqrt{10} + 10\sqrt{13}\right) - \left(6\sqrt{5} + 12\sqrt{18}\right) < 0.$$

This completes the proof. ■

3 Main results

In this section, we determine the extremal elliptic Sombor index among connected chemical graphs that are unicyclic, bicyclic, tricyclic, trees. We will first examine unicyclic graphs. The family of all connected chemical unicyclic graphs of order n is denoted by $\mathcal{A}_n$.

Lemma 5. [12] *A connected unicyclic graph G of order n has at most two pendent vertices, if and only if G is one of the graphs described in Table 1.*

Theorem 5. *For any connected chemical unicyclic graph G of order $n \geq 6$, with $G \in \mathcal{A}_n$ and $G \notin \{A_1, A_2, A_3, A_4\}$, where A_i are described in Table 1,*

$$ESO(A_1) < ESO(A_2) < ESO(A_3) < ESO(A_4) < ESO(G).$$

Proof. Based on Table 1, we have

$$ESO(A_1) < ESO(A_2) < ESO(A_3) < ESO(A_4).$$

Let $G \in \mathcal{A}_n$. If $n_1(G) \leq 2$, the result holds. If $n_1(G) \geq 3$, then by repeatedly applying Operations 1 and 3, we can construct a chemical unicyclic graph G^* that has exactly two pendent vertices. Consequently, using Lemmas 1 and 3, $ESO(G^*) < ESO(G)$. On the other hand, using Table 1, we have $ESO(A_4) \leq ESO(G^*)$ and therefore $ESO(A_4) < ESO(G)$. ■

Table 1. The chemical unicyclic graphs with $n_1 \leq 2$ sorted in ascending order of $ESO(G)$.

Graphs	m_{12}	m_{13}	m_{14}	m_{22}	m_{23}	m_{24}	m_{33}	$ESO \approx$
A_1	0	0	0	n	0	0	0	$8\sqrt{2}n$
A_2	0	1	0	$n-3$	2	0	0	$8\sqrt{2}n + 14.764$
A_3	1	0	0	$n-4$	3	0	0	$8\sqrt{2}n + 15.536$
A_4	0	2	0	$n-6$	4	0	0	$8\sqrt{2}n + 29.527$
A_5	0	2	0	$n-5$	2	0	1	$8\sqrt{2}n + 30.241$
A_6	1	1	0	$n-7$	5	0	0	$8\sqrt{2}n + 30.300$
A_7	1	1	0	$n-6$	3	0	1	$8\sqrt{2}n + 31.014$
A_8	2	0	0	$n-8$	6	0	0	$8\sqrt{2}n + 31.073$
A_9	2	0	0	$n-7$	4	0	1	$8\sqrt{2}n + 31.787$
A_{10}	0	0	2	$n-4$	0	2	0	$8\sqrt{2}n + 49.642$
A_{11}	1	0	1	$n-5$	0	3	0	$8\sqrt{2}n + 51.254$
A_{12}	2	0	0	$n-6$	0	4	0	$8\sqrt{2}n + 52.865$

The family of all connected chemical bicyclic graphs of order n is denoted by $\mathcal{B}_n$.

Lemma 6. [12] *A connected bicyclic graph G of order n has at most one pendent vertex, if and only if G is one of the graphs described in Table 2.*

Theorem 6. *Let G be a connected chemical bicyclic graph with $n \geq 6$. Assume that $G \in \mathcal{B}_n \setminus \{B_1, B_2, B_3\}$, where B_i are described in Table 2. Then*

$$ESO(B_1) < ESO(B_2) < ESO(B_3) < ESO(G).$$

Proof. Based on Table 2, we have

$$ESO(B_1) < ESO(B_2) < ESO(B_3).$$

Let $G \in \mathcal{B}_n$ of order $n \geq 6$. If $n_1(G) \leq 1$, the result holds. If $n_1(G) \geq 2$, then by repeatedly applying Operations 1 and 3, we can construct a chemical bicyclic graph G^* that has exactly one pendent vertex. Consequently, by using Lemmas 1 and 3, $ESO(G^*) < ESO(G)$. On the other hand, using Table 2, we have $ESO(B_3) \leq ESO(G^*)$ and therefore $ESO(B_3) < ESO(G)$. ■

Table 2. The chemical bicyclic graphs with $n_1 \leq 1$ sorted in ascending order of $ESO(G)$.

Graphs	m_{12}	m_{13}	m_{14}	m_{22}	m_{23}	m_{24}	m_{33}	m_{34}	$ESO \approx$
B_1	0	0	0	$n-5$	6	0	0	0	$8\sqrt{2}n + 51.599$
B_2	0	0	0	$n-4$	4	0	1	0	$8\sqrt{2}n + 52.312$
B_3	0	1	0	$n-8$	8	0	0	0	$8\sqrt{2}n + 66.362$
B_4	0	1	0	$n-7$	6	0	1	0	$8\sqrt{2}n + 67.077$
B_5	1	0	0	$n-9$	9	0	0	0	$8\sqrt{2}n + 67.135$
B_6	0	1	0	$n-6$	4	0	2	0	$8\sqrt{2}n + 67.790$
B_7	1	0	0	$n-8$	7	0	1	0	$8\sqrt{2}n + 67.849$
B_8	0	1	0	$n-5$	2	0	3	0	$8\sqrt{2}n + 68.504$
B_9	1	0	0	$n-7$	5	0	2	0	$8\sqrt{2}n + 68.563$
B_{10}	1	0	0	$n-6$	3	0	3	0	$8\sqrt{2}n + 69.283$
B_{11}	0	0	0	$n-3$	0	4	0	0	$8\sqrt{2}n + 73.390$
B_{12}	0	0	1	$n-6$	3	3	0	0	$8\sqrt{2}n + 87.314$
B_{13}	0	0	1	$n-5$	2	2	0	1	$8\sqrt{2}n + 88.770$
B_{14}	1	0	0	$n-7$	3	4	0	0	$8\sqrt{2}n + 88.923$
B_{15}	1	0	0	$n-6$	2	3	0	1	$8\sqrt{2}n + 90.382$

The family of all connected chemical tricyclic graphs of order n is denoted by $\mathcal{C}_n$.

Lemma 7. [12] *A connected tricyclic graph G of order n has at most one pendent vertex, if and only if G is one of the graphs described in Table 3.*

Theorem 7. *Let G be a connected chemical tricyclic graph with $n \geq 10$. Assume that $G \in \mathcal{C}_n \setminus \{C_1, C_2, C_3, C_4\}$, where C_i are described in Table 3. Then*

$$ESO(C_1) < ESO(C_2) < ESO(C_3) < ESO(C_4) < ESO(G).$$

Proof. Based on Table 3, we have

$$ESO(C_1) < ESO(C_2) < ESO(C_3) < ESO(C_4).$$

Let $G \in \mathcal{C}_n$ of order $n \geq 10$. If $n_1(G) \leq 1$, the result holds. If $n_1(G) \geq 2$, then by repeatedly applying Operations 1 and 3, we can construct a chemical tricyclic graph G^* that has exactly one pendent vertex. Consequently, by using Lemmas 1 and 3, $ESO(G^*) < ESO(G)$. On the other hand, using Table 2, we have $ESO(C_4) \leq ESO(G^*)$ and therefore $ESO(C_4) < ESO(G)$. ■

Next we investigate the extremal elliptic Sombor index of the family of chemical trees denoted by $\mathcal{T}_n$. We define two classes of chemical trees as follows.

- Let $\mathcal{T}_n^4$ be a class of chemical trees of order $n \geq 6$ with degree sequence $(4, \underbrace{2, \ldots, 2}_{\text{n-5}}, 1, 1, 1, 1)$ such that $m_{12} = m_{24} = 1$, $m_{14} = 3$ and $m_{22} = n - 6$.
- Let $\mathcal{T}_n^3$ be a class of chemical trees of order $n \geq 8$ with degree sequence $(3, 3, 3, \underbrace{2, \ldots, 2}_{\text{n-8}}, 1, 1, 1, 1, 1)$ such that $m_{13} = 5$, $m_{23} = 4$ and $m_{22} = n - 10$.

From the definition of the elliptic Sombor index, for any $T \in \mathcal{T}_n^4$ and $T' \in \mathcal{T}_n^3$, we can easily obtain

$$ESO(T) = 8\sqrt{2}n + 15\sqrt{5} + 15\sqrt{17} - 48\sqrt{2} \approx 8\sqrt{2}n + 27.505,$$

and

$$ESO(T') = 8\sqrt{2}n + 20\sqrt{10} + 20\sqrt{13} - 80\sqrt{2} \approx 8\sqrt{2}n + 22.220.$$

Theorem 8. *Let T be a chemical tree of order $n \geq 6$ with $\Delta = 4$. Then*

$$ESO(T) \geq 8\sqrt{2}n + 15\sqrt{5} + 15\sqrt{17} - 48\sqrt{2}.$$

Equality holds if and only if $T \in \mathcal{T}_n^4$.

Proof. Define $\mathcal{D} = (4, \underbrace{2, \ldots, 2}_{\text{n-5}}, 1, 1, 1, 1)$. We consider two following cases.

Case 1: Let $T \in \mathcal{T}_n$ with the degree sequence $\mathcal{D}$. If $T \in \mathcal{T}_n^4$, then the equality holds. If $T \notin \mathcal{T}_n^4$, then by repeatedly applying Operation 2, we can construct a chemical tree graph $T' \in \mathcal{T}_n^4$. Using Lemma 2, we have

$ESO(T') < ESO(T)$. Therefore, the proof is completed.

Case 2: Let $T \in \mathcal{T}_n$ does not have the degree sequence $\mathcal{D}$. In this case by repeated applications of Transformation 1, we obtain a chemical tree T' with the degree sequence $\mathcal{D}$.

If $T' \in \mathcal{T}_n^4$, then by Lemma 1, $ESO(T') < ESO(T)$. Otherwise, we follow the Case 1. ■

Table 3. The chemical tricyclic graphs with $n_1 \leq 1$ sorted in ascending order of $ESO(G)$.

Graphs	m_{12}	m_{13}	m_{14}	m_{22}	m_{23}	m_{24}	m_{33}	m_{34}	m_{44}	$ESO(G) \approx$
C_1	0	0	0	$n-10$	12	0	0	0	0	$8\sqrt{2}n + 103.197$
C_2	0	0	0	$n-9$	10	0	1	0	0	$8\sqrt{2}n + 103.911$
C_3	0	0	0	$n-8$	8	0	2	0	0	$8\sqrt{2}n + 104.624$
C_4	0	0	0	$n-7$	6	0	3	0	0	$8\sqrt{2}n + 105.338$
C_5	0	0	0	$n-6$	4	0	4	0	0	$8\sqrt{2}n + 106.051$
C_6	0	0	0	$n-5$	2	0	5	0	0	$8\sqrt{2}n + 106.765$
C_7	0	1	0	$n-13$	14	0	0	0	0	$8\sqrt{2}n + 117.963$
C_8	0	1	0	$n-12$	12	0	1	0	0	$8\sqrt{2}n + 118.675$
C_9	1	0	0	$n-14$	15	0	0	0	0	$8\sqrt{2}n + 118.735$
C_{10}	0	1	0	$n-11$	10	0	2	0	0	$8\sqrt{2}n + 119.387$
C_{11}	1	0	0	$n-13$	13	0	1	0	0	$8\sqrt{2}n + 119.449$
C_{12}	0	1	0	$n-10$	8	0	3	0	0	$8\sqrt{2}n + 120.101$
C_{13}	1	0	0	$n-12$	11	0	2	0	0	$8\sqrt{2}n + 120.162$
C_{14}	0	1	0	$n-9$	6	0	4	0	0	$8\sqrt{2}n + 120.815$
C_{15}	1	0	0	$n-11$	9	0	3	0	0	$8\sqrt{2}n + 120.875$
C_{16}	0	1	0	$n-8$	4	0	5	0	0	$8\sqrt{2}n + 121.529$
C_{17}	1	0	0	$n-10$	7	0	4	0	0	$8\sqrt{2}n + 121.588$
C_{18}	0	1	0	$n-7$	2	0	6	0	0	$8\sqrt{2}n + 122.243$
C_{19}	1	0	0	$n-9$	5	0	5	0	0	$8\sqrt{2}n + 122.302$
C_{20}	1	0	0	$n-8$	3	0	6	0	0	$8\sqrt{2}n + 123.017$
C_{21}	1	0	0	$n-7$	1	0	7	0	0	$8\sqrt{2}n + 123.729$
C_{22}	0	0	0	$n-8$	6	4	0	0	0	$8\sqrt{2}n + 124.990$
C_{23}	0	0	0	$n-7$	4	4	1	0	0	$8\sqrt{2}n + 125.703$
C_{24}	0	0	1	$n-6$	1	1	3	2	0	$8\sqrt{2}n + 125.934$
C_{25}	0	0	0	$n-7$	5	3	0	1	0	$8\sqrt{2}n + 126.442$
C_{26}	0	0	0	$n-6$	3	3	1	1	0	$8\sqrt{2}n + 127.156$
C_{27}	0	0	0	$n-6$	4	2	0	2	0	$8\sqrt{2}n + 127.895$
C_{28}	0	0	0	$n-5$	2	2	1	2	0	$8\sqrt{2}n + 128.608$
C_{29}	0	0	1	$n-11$	9	3	0	0	0	$8\sqrt{2}n + 138.915$
C_{30}	0	0	1	$n-10$	7	3	1	0	0	$8\sqrt{2}n + 139.629$
C_{31}	0	0	1	$n-9$	5	3	2	0	0	$8\sqrt{2}n + 140.342$
C_{32}	0	0	1	$n-10$	8	2	0	1	0	$8\sqrt{2}n + 140.367$
C_{33}	1	0	0	$n-12$	9	4	0	0	0	$8\sqrt{2}n + 140.527$
C_{34}	0	0	1	$n-8$	3	3	3	0	0	$8\sqrt{2}n + 141.057$
C_{35}	0	0	1	$n-9$	6	2	1	1	0	$8\sqrt{2}n + 141.082$
C_{36}	1	0	0	$n-9$	4	3	2	1	0	$8\sqrt{2}n + 141.240$
C_{37}	0	0	1	$n-8$	4	2	2	1	0	$8\sqrt{2}n + 141.795$

Graphs	m_{12}	m_{13}	m_{14}	m_{22}	m_{23}	m_{24}	m_{33}	m_{34}	m_{44}	$ESO(G) \approx$
C_{38}	0	0	1	$n-9$	7	1	0	2	0	$8\sqrt{2}n + 141.821$
C_{39}	1	0	0	$n-10$	5	4	2	0	0	$8\sqrt{2}n + 141.953$
C_{40}	1	0	0	$n-11$	8	3	0	1	0	$8\sqrt{2}n + 141.978$
C_{41}	0	0	1	$n-7$	2	2	3	1	0	$8\sqrt{2}n + 142.509$
C_{42}	0	0	1	$n-8$	5	1	1	2	0	$8\sqrt{2}n + 142.535$
C_{43}	1	0	0	$n-9$	3	4	3	0	0	$8\sqrt{2}n + 142.668$
C_{44}	1	0	0	$n-10$	6	3	1	1	0	$8\sqrt{2}n + 142.693$
C_{45}	0	0	1	$n-7$	3	1	2	2	0	$8\sqrt{2}n + 143.248$
C_{46}	0	0	1	$n-8$	6	0	0	3	0	$8\sqrt{2}n + 143.274$
C_{47}	1	0	0	$n-9$	4	3	2	1	0	$8\sqrt{2}n + 143.406$
C_{48}	1	0	0	$n-10$	7	2	0	2	0	$8\sqrt{2}n + 143.432$
C_{49}	0	0	1	$n-7$	4	0	1	3	0	$8\sqrt{2}n + 143.987$
C_{50}	1	0	0	$n-8$	2	3	3	1	0	$8\sqrt{2}n + 144.121$
C_{51}	1	0	0	$n-9$	5	2	1	2	0	$8\sqrt{2}n + 144.146$
C_{52}	0	0	1	$n-6$	2	0	2	3	0	$8\sqrt{2}n + 144.701$
C_{53}	1	0	0	$n-8$	3	2	2	2	0	$8\sqrt{2}n + 144.860$
C_{54}	1	0	0	$n-9$	6	1	0	3	0	$8\sqrt{2}n + 144.885$
C_{55}	1	0	0	$n-7$	1	2	3	2	0	$8\sqrt{2}n + 145.573$
C_{56}	1	0	0	$n-8$	4	1	1	3	0	$8\sqrt{2}n + 145.599$
C_{57}	1	0	0	$n-7$	2	1	2	3	0	$8\sqrt{2}n + 146.312$
C_{58}	0	0	0	$n-6$	0	8	0	0	0	$8\sqrt{2}n + 146.781$
C_{59}	1	0	0	$n-6$	0	1	3	3	0	$8\sqrt{2}n + 147.026$
C_{60}	0	0	0	$n-5$	0	6	0	0	1	$8\sqrt{2}n + 149.755$
C_{61}	0	0	1	$n-9$	3	7	0	0	0	$8\sqrt{2}n + 160.708$
C_{62}	0	0	1	$n-8$	2	6	0	1	0	$8\sqrt{2}n + 162.161$
C_{63}	1	0	0	$n-10$	3	8	0	0	0	$8\sqrt{2}n + 162.319$
C_{64}	0	0	1	$n-8$	3	5	0	0	1	$8\sqrt{2}n + 163.611$
C_{65}	0	0	1	$n-7$	1	5	0	2	0	$8\sqrt{2}n + 163.613$
C_{66}	1	0	0	$n-9$	2	7	0	1	0	$8\sqrt{2}n + 163.772$
C_{67}	0	0	1	$n-7$	2	4	0	1	1	$8\sqrt{2}n + 165.063$
C_{68}	1	0	0	$n-9$	3	6	0	0	1	$8\sqrt{2}n + 165.222$
C_{69}	1	0	0	$n-8$	1	6	0	2	0	$8\sqrt{2}n + 165.225$
C_{70}	0	0	1	$n-6$	1	3	0	2	1	$8\sqrt{2}n + 166.516$
C_{71}	1	0	0	$n-8$	2	5	0	1	1	$8\sqrt{2}n + 166.675$
C_{72}	1	0	0	$n-7$	1	4	0	2	1	$8\sqrt{2}n + 167.127$

Theorem 9. *Let T be a chemical tree of order $n \geq 10$ with $\Delta \leq 3$ such that $T \in \mathcal{T}_n \setminus \{T_i, \mathcal{T}_n^3\}$ where T_i for $1 \leq i \leq 12$ are described in Table 4. Then*

$$ESO(T_i) < ESO(T_{i+1}) < ESO(\mathcal{T}_n^3) < ESO(T).$$

Proof. Let $T \in \mathcal{T}_n$. Based on the number of vertices of degree 3, we consider two following cases.

Case 1: Let $n_3(T) \leq 2$. In such a case, the ESO index of all chemical trees with $\Delta \leq 3$ and $n_3(T) \leq 2$ are calculated in Table 4. Therefore, we have

Table 4. The chemical trees with $\Delta \leq 3$ and $n_3 \leq 2$.

Tree	m_{12}	m_{13}	m_{22}	m_{23}	m_{33}	ESO $\approx$
T_1	2	0	$n-3$	0	0	$8\sqrt{2}n - 20.525$
T_2	1	2	$n-5$	1	0	$8\sqrt{2}n - 6.535$
T_3	2	1	$n-6$	2	0	$8\sqrt{2}n - 5.761$
T_4	3	0	$n-7$	3	0	$8\sqrt{2}n - 4.988$
T_5	0	4	$n-7$	2	0	$8\sqrt{2}n + 7.456$
T_6	1	3	$n-8$	3	0	$8\sqrt{2}n + 8.229$
T_7	1	3	$n-7$	1	1	$8\sqrt{2}n + 8.943$
T_8	2	2	$n-9$	4	0	$8\sqrt{2}n + 9.002$
T_9	2	2	$n-8$	2	1	$8\sqrt{2}n + 9.716$
T_{10}	3	1	$n-10$	5	0	$8\sqrt{2}n + 9.775$
T_{11}	3	1	$n-9$	3	1	$8\sqrt{2}n + 10.489$
T_{12}	4	0	$n-11$	6	0	$8\sqrt{2}n + 10.548$
T_{13}	4	0	$n-10$	4	1	$8\sqrt{2}n + 11.263$

$ESO(T_i) < ESO(T_{i+1}) < ESO(\mathcal{T}_n^3)$ for $1 \leq i \leq 12$.
Case 2: Let $n_3(T) = 3$. If $T \in \mathcal{T}_n^3$, the result holds. If $T \notin \mathcal{T}_n^3$, then using Operations 2 and 4, we obtain a chemical tree $T^* \in \mathcal{T}_n^3$ such that $ESO(T^*) < ESO(T)$.
Case 3: Let $n_3(T) \geq 4$. By repeatedly applying Operation 1, we construct a chemical tree graph T^* whose degree sequence is $(3, 3, 3, \underbrace{2, \ldots, 2}_{n-8}, 1, 1, 1, 1, 1)$. Therefore using Lemma 1, we have $ESO(T^*) < ESO(T)$. If $T^* \in \mathcal{T}_n^3$, the result holds. If $T^* \notin \mathcal{T}_n^3$, then we follow Case 2. ■

4 Conclusion

In this paper, we investigated the behavior of the elliptic Sombor index within several important classes of chemical graphs and established the ordering of graphs with the minimum value of this index among chemical trees, chemical unicyclic graphs, chemical bicyclic graphs, and chemical tricyclic graphs. By introducing and systematically applying a family of graph transformations that strictly decrease the elliptic Sombor index, we characterized the corresponding extremal structures and provided explicit descriptions of the graphs that attain these minimal values. These results enhance the structural understanding of the elliptic Sombor index and clarify how local degree distributions and cycle structure influence its magnitude in chemically relevant graph classes. In addition to their intrinsic graph-theoretical interest, the obtained characterizations may serve as a theoretical basis for further applications of the elliptic Sombor index in QSPR/QSAR modeling, especially when identifying molecular structures that minimize or constrain this descriptor. It would be natural in future work to extend the present methods to broader families of chemical graphs with higher cyclomatic number, to other variants of Sombor-type indices, and to explore more systematically the interplay between extremal behavior of these indices and their predictive performance in chemical property modeling.

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