Communications in Combinatorics and Optimization
Vol. xx, No. x (xxxx), pp. 1-21
https://doi.org/10.22049/cco.2025.29344.1951

CCO
Commun. Comb. Optim.

Research Article

Extended Sombor Indices

Sultan Ahmad†, Rashid Farooq*

Department of Mathematics, School of Natural Sciences,
National University of Sciences and Technology, H-12, Islamabad 44000, Pakistan
†raosultan58@gmail.com
*farook.ra@gmail.com

Received: 9 January 2024; Accepted: 4 July 2025
Published Online: 17 July 2025

Abstract: In this paper, we present a novel perspective on vertex-degree-based topological indices. Established degree–based topological indices are based on adjacent vertices. One could contemplate including all pairs of vertices. Recently, Gutman introduced the Sombor indices. Here, we introduce the extended versions of the Sombor indices including all pairs of vertices in the Sombor indices formula. We explore the fundamental mathematical properties of these extended indices, establish upper and lower bounds in terms of some graph parameters, and find the sharp bounds. Additionally, we determine the extremal chemical trees with maximum and minimum extended Sombor index. Moreover, the role of extended Sombor indices in describing structure–property relationships is demonstrated.

Keywords: Sombor indices, extended Sombor indices, chemical trees.

AMS Subject classification: 05C09, 05C35

1. Introduction

Let G be a simple finite graph with vertex set $V(G)$ and edge set $E(G)$. The order and size of G are respectively denoted by $n(G)$ and $m(G)$. The edge between any two vertices u and v in G is written by uv (or vu). The degree of a vertex u in G is denoted by $d_u(G)$ and the set of its neighbors is denoted by $N_u(G)$. The maximum and minimum degree of G are respectively denoted by $\Delta(G)$ and $\delta(G)$. If $\Delta(G) = \delta(G)$, then G is called a regular graph. In graph G, a vertex with degree 1 is called a pendant vertex. A degree sequence is the list of vertex degrees in non-increasing order. A graph is called an acyclic graph if it has no cycles. A connected acyclic

* *Corresponding Author*

graph is called a tree. A tree in which all vertices have a maximum degree 4 is called a chemical tree. A chemical tree is the graphical representation of the carbon-atom structure of an alkane. Chemical trees have been extensively studied in the literature [5, 18, 20]. The complement graph $\overline{G}$ of G has the set of vertices $V(G)$ and $uv \in E(\overline{G})$ if and only if $uv \notin E(G)$. Note that $E(G) \cup E(\overline{G})$ represents the set of edges that belong to G and $\overline{G}$. Therefore, $|E(G) \cup E(\overline{G})| = \binom{n}{2}$. The degree of vertex u in $\overline{G}$ is given as $d_u(\overline{G}) = n - 1 - d_u(G)$. The number of vertices of degree i in G is denoted by $n_i(G)$ and the number of pairs of vertices of degree i and j in G is denoted by $c_{ij}(G)$. If the confusion is not a concern, we opt for d_u over $d_u(G)$, N_u over $N_u(G)$, Δ over $\Delta(G)$, δ over $\delta(G)$, n over $n(G)$ and m over $m(G)$, n_i over $n_i(G)$ and c_{ij} over $c_{ij}(G)$. Additional graph theory notions may be found in [13].

In theoretical chemistry, topological indices are highly valuable and they have been used as molecular descriptors due to their main characteristics, that is, their simple definitions, thus the ease of calculation and the considerable amount of structural information they are harvesting [33]. The most important applications of topological indices are in QSPR/QSAR modeling [10, 12]. So far, countless number of graph indices have been proposed, mostly belonging to the degree–, distance–, or eigenvalue–based group of indices, depending on their definitions. Topological indices have also been applied in graph algorithms and network communication [23].

Quite recently, a set of three degree–based graph indices have been introduced after geometric considerations of a graph. These are called Sombor indices [14]. Even though Sombor indices are new graph invariants, they have attracted enormous attention of both chemists and mathematicians. This resulted in a large number of published studies, see for example [1, 2, 4–9, 16, 18, 19, 21, 22, 24–27, 30, 31, 34]. The Sombor index (SO), the reduced Sombor index (SO_{red}), and the average Sombor index (SO_{avg}) of a graph G are respectively defined as:

$$\begin{aligned} SO(G) &= \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2} \\ SO_{red}(G) &= \sum_{uv \in E(G)} \sqrt{(d_u - 1)^2 + (d_v - 1)^2} \\ SO_{avg}(G) &= \sum_{uv \in E(G)} \sqrt{\left(d_u - 2m/n\right)^2 + \left(d_v - 2m/n\right)^2}. \end{aligned}$$

In the Sombor indices formulas, we see that only pairs of adjacent vertices are considered. One could contemplate including all pairs of vertices in the Sombor indices formulas. This results in the introduction of extended Sombor index (ESO), extended reduced Sombor index (ESO_{red}), and extended average Sombor index (ESO_{avg}) defined respectively as follows:

$$ESO(G) = \sum_{\substack{\{u,v\} \subseteq V(G) \\ u \neq v}} \sqrt{d_u^2 + d_v^2}$$

$$ESO_{red}(G) = \sum_{\substack{\{u,v\} \subseteq V(G) \\ u \neq v}} \sqrt{(d_u - 1)^2 + (d_v - 1)^2}$$

$$ESO_{avg}(G) = \sum_{\substack{\{u,v\} \subseteq V(G) \\ u \neq v}} \sqrt{\left(d_u - 2m/n\right)^2 + \left(d_v - 2m/n\right)^2}.$$

Remark 1. Let G and G^* be two non-isomorphic graphs, both having order n and the same degree sequence. Then it is obvious to see that $ESO(G) = ESO(G^*)$, $ESO_{red}(G) = ESO_{red}(G^*)$ and $ESO_{avg}(G) = ESO_{avg}(G^*)$.

The extended Sombor index of G can be restated as:

$$ESO(G) = \sum_{1 \leq i \leq j \leq \Delta} c_{ij} \sqrt{i^2 + j^2}. \tag{1.1}$$

The following is easy to verify for a graph G:

$$c_{ij} = c_{ji} = \begin{cases} n_i n_j & \text{if } i \neq j, \\ \binom{n_i}{2} & \text{if } i = j. \end{cases} \tag{1.2}$$

This paper is organized as follows: In section 2, we find the extremal graphs with respect to extended Sombor index. In section 3, we explore the basic mathematical features and establish the bounds (lower and upper) on ESO and ESO_{red} in terms of some graph parameters. In section 4, we find the extremal chemical trees of order n with maximum and minimum ESO index. In section 5, we demonstrate the chemical significance of extended Sombor indices. In section 6, we give the conclusion.

2. Extremal graphs with respect to extended Sombor index

In this section, we will find some extremal graphs with respect to the extended Sombor index. It is obvious to see that $ESO(K_n) = SO(K_n) = \dfrac{n(n-1)^2}{\sqrt{2}}$, $ESO_{red}(K_n) = SO_{red}(K_n) = \dfrac{n(n-1)(n-2)}{\sqrt{2}}$ and $ESO_{avg}(K_n) = SO_{avg}(K_n) = 0$. For any graph G of order n, we obtain

$$0 \leq ESO(G) \leq ESO(K_n).$$

The right inequality (left inequality) turns into equality if and only if $G \cong K_n$ ($G \cong \overline{K_n}$).

We will now establish the upper and lower bounds on extended Sombor indices for complete graph K_n, path graph P_n, star graph S_n and tree T of order n. First, we consider the following two useful results, which will be frequently employed in the subsequent result.

Lemma 1. *Let $f(x,y) = \sqrt{(x-1)^2+y^2} - \sqrt{x^2+y^2}$, where $x > 1$ and $y > 0$. Then $f(x,y)$ is a strictly decreasing function on x and strictly increasing on y.*

Proof. We obtain

$$f'_x(x,y) = \frac{(x-1)\sqrt{x^2+y^2} - x\sqrt{(x-1)^2+y^2}}{\sqrt{\Big((x-1)^2+y^2\Big)(x^2+y^2)}}.$$

Note that $(x-1)^2(x^2+y^2) - x^2\Big((x-1)^2+y^2\Big) = -y^2(2x-1) < 0$ for $x > 1$ and $y > 0$. This gives $(x-1)\sqrt{x^2+y^2} < x\sqrt{(x-1)^2+y^2}$ for $x > 1$ and $y > 0$. Hence $f'_x(x,y) < 0$. So $f(x,y)$ is a strictly decreasing function on x.

For $x > 1$ and $y > 0$, we obtain

$$f'_y(x,y) = \frac{y}{\sqrt{(x-1)^2+y^2}} - \frac{y}{\sqrt{x^2+y^2}} < 0.$$

So $f(x,y)$ is a strictly decreasing function on y. This completes the proof. □

We introduce two graph transformations in the following lemmas, which either increase or decrease the ESO index.

Lemma 2. *Let G be a connected graph, and consider $u, v_1 \in V(G)$ and $v_1v_2 \in E(G)$, where $d_u(G) = p \geq 3$, $d_{v_1} = 1$ and $d_{v_2} \geq 2$. Assume u_1 is a neighbor of u such that u_1 is not on u, v_1-path. Let G^* be the graph obtained from G such that $G^* = G - \{uu_1\} + \{u_1v_1\}$. Then $ESO(G^*) < ESO(G)$.*

Proof. Note that $d_u(G^*) = p-1$, $d_{v_1}(G^*) = d_{v_1}(G)+1 = 2$ and $d_v(G^*) = d_v(G)$ for all $v \in V(G)\backslash\{u_1, v_1\}$. Let $U = V(G)\backslash\{\{u\} \cup \{w \in V(T) \mid d_w(G) = 1\}\}$ and $r = |U|$. We obtain

$$\begin{aligned} ESO(G^*) - ESO(G) = {} & \sqrt{(p-1)^2+4} - \sqrt{p^2+1} + (n_1-1)\Bigg(\sqrt{(p-1)^2+1} - \sqrt{p^2+1} \\ & + \sqrt{5} - \sqrt{2}\Bigg) + \sum_{v \in U}\Bigg(\sqrt{(p-1)^2+d_v^2} - \sqrt{p^2+d_v^2} + \sqrt{4+d_v^2} \\ & - \sqrt{1+d_v^2}\Bigg). \end{aligned}$$

$$ESO(G^*) - ESO(G) < (n_1 - 1)\Big(\sqrt{(p-1)^2+1} - \sqrt{p^2+1} + \sqrt{5} - \sqrt{2}\Big)$$
$$+ \sum_{v \in U}\Big(\sqrt{(p-1)^2+d_v^2} - \sqrt{p^2+d_v^2} + \sqrt{4+d_v^2} - \sqrt{1+d_v^2}\Big)$$

Since $p \geq 3$, using Lemma 1 we have $f(p,1) \leq f(3,1)$ and $f(p,d_v) \leq f(3,d_v)$. Then

$$\begin{aligned} ESO(G^*) - ESO(G) &< (n_1-1)\Big(\sqrt{5} - \sqrt{10} + \sqrt{5} - \sqrt{2}\Big) + r\Big(2\sqrt{4+d_v^2} - \sqrt{9+d_v^2} \\ &\quad - \sqrt{1+d_v^2}\Big) \\ &= -0.1(n_1-1) + +r\Big(2\sqrt{4+d_v^2} - \sqrt{9+d_v^2} - \sqrt{1+d_v^2}\Big). \end{aligned}$$

Since $4 \cdot d_v^2 > 0$, it follows that $(d_v^4 + 10d_v^2 + 9) > (d_v^2+3)^2$, that is, $\sqrt{9+d_v^2} + \sqrt{1+d_v^2} > 2\sqrt{4+d_v^2}$. This means $ESO(G^*) - ESO(G) < 0$, which completes the proof. □

Lemma 3. *Let G be a connected graph, and consider $u, v_1 \in V(G)$, where $d_u(G) = \Delta \geq 3$ and $d_{v_1} \geq 2$. Assume v_2 is a neighbor of v_1 such that v_2 is not on u, v_1-path. Let G^* be a graph obtained from G such that $G^* = G - \{v_1v_2\} + \{uv_2\}$. Then $ESO(G^*) > ESO(G)$.*

Proof. Note that $d_u(G^*) = \Delta + 1$, $d_{v_1}(G^*) = d_{v_1}(G) - 1$ and $d_v(G^*) = d_v(G)$ for all $v \in V(G) \backslash \{u, v_1\}$. Let $U = V(G) - \{\{u, v_1\} \cup \{w \in V(G) \mid d_w(G) = 1\}\}$ and $r = |U|$. Then

$$\begin{aligned} ESO(G^*) - ESO(G) &= \sqrt{(\Delta+1)^2 + (d_{v_1}-1)^2} - \sqrt{\Delta^2 + d_{v_1}^2} + n_1\Big(\sqrt{(\Delta+1)^2+1} \\ &\quad - \sqrt{\Delta^2+1} + \sqrt{(d_{v_1}-1)^2+1} - \sqrt{d_{v_1}^2+1}\Big) + \sum_{v\in U}\Big(\sqrt{(d_{v_1}-1)^2+d_v^2} \\ &\quad - \sqrt{d_{v_1}^2+d_v^2} + \sqrt{(\Delta+1)^2+d_v^2} - \sqrt{\Delta^2+d_v^2}\Big). \end{aligned}$$

Note that

$$\sqrt{(\Delta+1)^2 + (d_{v_1}-1)^2} - \sqrt{\Delta^2 + d_{v_1}^2} = \sqrt{\Delta^2 + d_{v_1}^2 + 2 + 2(\Delta - d_{v_1})} - \sqrt{\Delta^2 + d_{v_1}^2} > 0.$$

Then

$$\begin{aligned} ESO(G^*) - ESO(G) &> n_1\Big(\sqrt{(\Delta+1)^2+1} - \sqrt{\Delta^2+1} + \sqrt{(d_{v_1}-1)^2+1} - \sqrt{d_{v_1}^2+1}\Big) \\ &\quad + \sum_{v\in C}\Big(\sqrt{(d_{v_1}-1)^2+d_v^2} - \sqrt{d_{v_1}^2+d_v^2} + \sqrt{(\Delta+1)^2+d_v^2} - \sqrt{\Delta^2+d_v^2}\Big). \end{aligned}$$

Since $\Delta \geq d_{v_1} \geq 2$, using Lemma 1, we have $f(d_{v_1}, 1) \geq f(\Delta, 1)$ and $f(d_{v_1}, d_v) \geq f(\Delta, d_v)$. Then, from the above, we obtain

$$\begin{aligned} ESO(G^*) - ESO(G) > n_1\bigg(\sqrt{(\Delta+1)^2+1} + \sqrt{(\Delta-1)^2+1} - 2\sqrt{\Delta^2+1}\bigg) \\ + r\bigg(\sqrt{(\Delta+1)^2+d_v^2} + \sqrt{(\Delta-1)^2+d_v^2} - 2\sqrt{\Delta^2+d_v^2}\bigg). \end{aligned} \tag{2.1}$$

One can easily check that $(\Delta^2 + 2\Delta + 2)(\Delta^2 - 2\Delta + 2) > \Delta^4$, that is,

$$\sqrt{(\Delta+1)^2+1} + \sqrt{(\Delta-1)^2+1} > 2\sqrt{\Delta^2+1}.$$

Similarly, one can obtain

$$2 + 2\cdot d_v^2 + 2\sqrt{\Big((\Delta+1)^2+d_v^2\Big)\Big((\Delta-1)^2+d_v^2\Big)} > 0, \quad \text{that is,}$$
$$2\left[1 + \sqrt{\Big((\Delta+1)^2+d_v^2\Big)\Big((\Delta-1)^2+d_v^2\Big)}\right] > 2(\Delta^2+d_v^2),$$

that is,

$$\sqrt{(\Delta+1)^2+d_v^2} + \sqrt{(\Delta-1)^2+d_v^2} > -2\sqrt{\Delta^2+d_v^2}.$$

Thus, from (2.1), we obtain

$$ESO(G^*) - ESO(G) > 0,$$

completing the proof. □

Theorem 1. *Let G be a connected graph of order n. Then we have*

$$ESO(P_n) \leq ESO(G) \leq ESO(K_n).$$

The left inequality (right inequality) turns into equality if and only if $G \cong P_n$ ($G \cong K_n$). In addition, $ESO(P_n) = \sqrt{2}(n^2 - 5n + 7) + 2(n-2)\sqrt{5}$.

Proof. The upper bound is straightforward. To obtain the lower bound, observe that deleting edges from a graph G decreases its ESO index. Therefore, the minimum ESO index is attained by an n-vertex tree. Now assume for contradiction that $T \ncong P_n$ has the minimum ESO index among all trees of order n. Then there exist distinct vertices u and v_1 in G such that $d_u(T) = p \geq 3$ and $d_{v_1}(T) = 1$. Let u_1 be the neighbor of u that is not on u, v_1-path. We construct a tree T^* from G as follows: $G^* = G - uu_1 + u_1v_1$. By Lemma 2, it follows that $ESO(T^*) < ESO(T)$, which contradicts our assumption. Therefore, P_n has the minimum ESO index among all the trees of order n. This completes our result. □

Theorem 2. *Let T be a tree of order $n \geq 4$. Then we have*

$$ESO(P_n) \leq ESO(T) \leq ESO(S_n).$$

The left inequality (right inequality) turns into equality if and only if $T \cong P_n$ ($T \cong S_n$). In addition, $ESO(S_n) = (n-1)\left[\dfrac{n-2}{\sqrt{2}} + \sqrt{n^2 - 2n + 2}\right]$.

Proof. The lower bound follows from Theorem 1. To obtain the upper bound, suppose on contrary that $T \ncong S_n$ has the maximum ESO index among all trees of order $n \geq 4$. Then there exist distinct vertices u and v_1 in T such that $d_u(T) = \Delta \geq 3$ and $d_{v_1}(T) \geq 2$. Let v_2 be the neighbor of v_1 that is not on u, v_1-path. We construct a tree T^* from T as follows: $T^* = T - v_1v_2 + uv_2$. By Lemma 3, it follows that $ESO(T^*) > ESO(T)$, which contradicts our assumption. Therefore, S_n has the maximum ESO index among all the trees of order n. This completes our result. □

3. Bounds on extended Sombor indices of graphs

In this section, we establish bounds (lower and upper) on extended Sombor indices in terms of order, size, maximum degree, and minimum degree of graphs. From [15, 35], the following inequalities are immediate.
For non-negative real numbers $\mu_1 > 0$ and $\mu_2 > 0$ (or $\mu_1 > 1$ and $\mu_2 > 1$), we have (3.1) (or (3.2)) as follows:

$$\frac{1}{\sqrt{2}}(\mu_1 + \mu_2) \leq \sqrt{\mu_1^2 + \mu_2^2} < \mu_1 + \mu_2. \tag{3.1}$$

$$\frac{1}{\sqrt{2}}(\mu_1 + \mu_2 - 2) \leq \sqrt{(\mu_1 - 1)^2 + (\mu_2 - 1)^2} < (\mu_1 + \mu_2 - 2). \tag{3.2}$$

The left inequalitis in (3.1) and (3.2) turn into equalities if and only if $\mu_1 = \mu_2$.

Theorem 3. *Let G be a connected graph of order n and size m. Then*

$$(i) \qquad \binom{n}{2}\frac{n\delta^2}{\sqrt{2}m} \leq ESO(G) < \binom{n}{2}\frac{n\Delta^2}{m},$$

$$(ii) \qquad \binom{n}{2}\frac{n(\delta-1)\delta}{\sqrt{2}m} \leq ESO_{red}(G) < \binom{n}{2}\frac{n(\Delta-1)\Delta}{m}.$$

In both (i) and (ii), the left inequalities turn into equalities if and only if G is a regular graph.

Proof. (i) With summation over all pairs of vertices, we derive the following from right inequality in (3.1).

$$ESO(G) < \sum_{\substack{\{u,v\}\subseteq V(G)\\ u\neq v}} (d_u + d_v). \tag{3.3}$$

Since $\delta \leq d_u \leq \Delta$, for each $u \in V(G)$, it follows that

$$\sum_{\substack{\{u,v\}\subseteq V(G)\\ u\neq v}} (d_u + d_v) \leq \tbinom{n}{2} 2\Delta. \tag{3.4}$$

From the handshaking lemma, we have

$$n\delta \leq \sum_{u\in V(G)} d_u = 2m \leq n\Delta. \tag{3.5}$$

The inequalities in (3.5) turn into equalities if and only if G is a regular graph. By using (3.4) and (3.5) in (3.3), we obtain

$$ESO(G) < \tbinom{n}{2}\frac{n\Delta^2}{m}.$$

Similarly, using the left inequalities in (3.1) and (3.5), we obtain $\tbinom{n}{2}\dfrac{n\delta^2}{\sqrt{2}m} \leq ESO(G)$ and it turns into equality if and only if $d_u = \delta$ for each $u \in V(G)$, implying G is a regular graph.
(ii) The proof is analogous to (i), utilizing (3.2). $\square$

Since $\Delta \leq n-1$, we get the following corollary.

Corollary 1. *Let G be a connected graph of order n. Then*

$$(i) \qquad ESO(G) < \frac{n^2(n-1)^3}{2m},$$
$$(ii) \qquad ESO_{red}(G) < \frac{n^2(n-1)^2(n-2)}{2m}.$$

Lemma 4. [3] Let G be a graph of order n and size m. Then

$$\sum_{\substack{\{u,v\}\subseteq V(G)\\ u\neq v}} (d_u + d_v) = 2m(n-1).$$

Theorem 4. *Let G be a connected graph of order n and size m. Then*

$$(i) \qquad \sqrt{2}m(n-1) \leq ESO(G) < 2m(n-1),$$
$$(ii) \qquad \frac{(n-1)(2m-n)}{\sqrt{2}} \leq ESO_{red}(G) < (n-1)(2m-n).$$

In both (i) and (ii), the left inequalities turn into equalities if and only if G is a regular graph.

Proof. (i) With summation over all pairs of vertices, we derive the following from left inequality in (3.1).

$$ESO(G) \geq \frac{1}{\sqrt{2}} \sum_{\substack{\{u,v\} \subseteq V(G) \\ u \neq v}} (d_u + d_v).$$

By using Lemma 4, we obtain

$$ESO(G) \geq \sqrt{2}m(n-1).$$

Moreover, the left inequality in (i) turns into equality if and only if $d_u = d_v$ for any $\{u, v\} \subseteq V(G)$, implying G is a regular graph. Similarly, using the right inequality in (3.1) and Lemma 4, we obtain $ESO(G) < 2m(n-1)$. In addition, the proof of (ii) is analogous to (i), utilizing (3.2). □

Lemma 5. [35] Let G be a connected graph of order n. Then

$$SO(G) \leq \sqrt{2}m(n-1).$$

The inequality turns into equality if and only if $G \cong K_n$.

From Lemma 5 and left inequality in Theorem 4 (i), we have the following corollary.

Corollary 2. *Let G be a connected graph of order n. Then*

$$SO(G) \leq ESO(G).$$

The inequality turns into equality if and only if $G \cong K_n$.

The following result is straightforward.

Lemma 6. *Let $f(x) = (x-a)^2 + (n-x-a)^2$, where $1 \leq x \leq n$ and $a \geq 0$. Then $f(x)$ is decreasing for $1 \leq x \leq \frac{n}{2}$ and increasing for $\frac{n}{2} \leq x \leq n$.*

Theorem 5. *Let G be an acyclic graph of order n. Then*

$$(i) \qquad ESO(G) \leq \begin{cases} \binom{n}{2}\sqrt{\delta^2 + (n-\delta)^2} & \text{if } \Delta + \delta \leq n, \\ \binom{n}{2}\sqrt{\Delta^2 + (n-\Delta)^2} & \text{if } \Delta + \delta \geq n, \end{cases}$$

$$(ii) \qquad ESO_{red}(G) \leq \begin{cases} \binom{n}{2}\sqrt{(\delta-1)^2 + (n-\delta-1)^2} & \text{if } \Delta + \delta \leq n, \\ \binom{n}{2}\sqrt{(\Delta-1)^2 + (n-\Delta-1)^2} & \text{if } \Delta + \delta \geq n. \end{cases}$$

Proof. (i) Since G is an acyclic graph, for any $\{u,v\} \subseteq V(G)$, it holds $d_u + d_v \leq n$. Then

$$ESO(G) \leq \sum_{\substack{\{u,v\}\subseteq V(G) \\ u\neq v}} \sqrt{d_u^2 + (n-d_u)^2}.$$

From Lemma 6, it can be seen that

$$\begin{aligned} ESO(G) &\leq \sum_{\substack{\{u,v\}\subseteq V(G) \\ u\neq v}} \sqrt{d_u^2 + (n-d_u)^2} \\ &\leq \begin{cases} \binom{n}{2}\sqrt{\delta^2 + (n-\delta)^2} & \textit{if} \ \ \Delta+\delta \leq n, \\ \binom{n}{2}\sqrt{\Delta^2 + (n-\Delta)^2} & \textit{if} \ \ \Delta+\delta \geq n. \end{cases} \end{aligned}$$

This completes the proof of (i). The proof of (ii) is analogous to (i), utilizing Lemma 6. □

Theorem 6. *Let G be a connected graph of order n and size m. Then*

$$\begin{aligned} &(i) \qquad \binom{n}{2}\frac{n\delta^2}{\sqrt{2}m} \leq ESO(G) \leq \binom{n}{2}\frac{n\Delta^2}{\sqrt{2}m}, \\ &(ii) \qquad \binom{n}{2}\frac{n\delta(\delta-1)}{\sqrt{2}m} \leq ESO_{red}(G) \leq \binom{n}{2}\frac{n\Delta(\Delta-1)}{\sqrt{2}m}. \end{aligned}$$

The left and right inequalities in (i) and (ii) turn into equalities if and only if G is a regular graph.

Proof. (i) Since $\delta \leq d_u \leq \Delta$, for each $u \in V(G)$, it holds that

$$ESO(G) = \sum_{\substack{\{u,v\}\subseteq V(G) \\ u\neq v}} \sqrt{d_u^2 + d_v^2} \geq \binom{n}{2}\sqrt{2}\delta,$$

By using (3.5), we obtain

$$ESO(G) \geq \binom{n}{2}\frac{n\delta^2}{\sqrt{2}m}.$$

Furthermore, the left inequality in (i) turns into equality if and only if $d_u = \delta$ for each $u \in V(G)$, implying G is a regular graph. Similarly, the right inequality in (i) holds and turns into equality if and only if $d_u = \Delta$ for each $u \in V(G)$, implying G is a regular graph. In addition, the proof of (ii) is analogous to (i). □

Since $\Delta \leq n-1$, we get the following corollary.

Corollary 3. *Let G be a connected graph of order n and size m. Then*

$$\begin{aligned}
(i) \qquad & ESO(G) \le \frac{n(n-1)}{2m} ESO(K_n), \\
(ii) \qquad & ESO_{red}(G) \le \frac{n(n-1)}{2m} ESO_{red}(K_n).
\end{aligned}$$

The inequalities in (i) and (ii) turn into equalities if and only if $G \cong K_n$

Theorem 7. *Let $\overline{G}$ be the complement graph of a connected graph G with order n. Then*

$$\binom{n}{2}\frac{n\delta}{\sqrt{2}m}(n-1-\Delta) \le ESO(\overline{G}) \le \binom{n}{2}\frac{n\Delta}{\sqrt{2}m}(n-1-\delta).$$

The left and right inequality turns into equality if and only if G is a regular graph.

Proof. The extended Sombor index for $\overline{G}$ is defined as:

$$ESO(\overline{G}) = \sum_{\substack{\{u,v\}\subseteq V(\overline{G}) \\ u\neq v}} \sqrt{d_u^2(\overline{G}) + d_v^2(\overline{G})}.$$

Since $d_u(\overline{G}) = n-1-d_u(G)$ and $\delta \le d_u(G) \le \Delta$, for each $u \in V(G)$, it holds that

$$ESO(\overline{G}) \le \binom{n}{2}\sqrt{2}(n-1-\delta).$$

By using (3.5), we obtain

$$ESO(\overline{G}) \le \binom{n}{2}\frac{n\Delta}{\sqrt{2}m}(n-1-\delta).$$

Furthermore, the right inequality turns into equality if and only if $d_u(G) = \Delta$ for each $u \in V(G)$, implying G is a regular graph. Similarly, the left inequality holds and turns into equality if and only if $d_u(G) = \delta$ for each $u \in V(G)$, implying G is a regular graph. □

From Theorems 6 (i) and 7, we get the following corollary.

Corollary 4. *Let $\overline{G}$ be the complement graph of a connected graph G with order n. Then*

$$\binom{n}{2}\frac{n\delta}{\sqrt{2}m}(\delta+n-1-\Delta) \le ESO(G)+ESO(\overline{G}) \le \binom{n}{2}\frac{n\Delta}{\sqrt{2}m}(n+\Delta-1-\delta).$$

The left and right inequalities turn into equalities if and only if G is a regular graph.

We now establish upper bounds on ESO and ESO_{red} in terms of order only.

Theorem 8. *Let G be a connected graph of order. Then*

$$\begin{array}{ll} (i) & ESO(G) < \binom{n}{2}(2n-2), \\ (ii) & ESO_{red}(G) < 2\binom{n}{2}(n-2). \end{array}$$

Proof. (i) From (3.3), it follows that

$$ESO(G) < \sum_{\substack{\{u,v\}\subseteq V(G)\\ u\neq v}} (d_u + d_v).$$

Since $d_u \leq n-1$, for any $\{u,v\} \subseteq V(G)$, it holds $d_u + d_v \leq 2n-2$. Thus

$$\sum_{\substack{\{u,v\}\subseteq V(G)\\ u\neq v}} (d_u + d_v) \leq \binom{n}{2}(2n-2).$$

This completes the proof of (i). Analogously, the inequality (ii) is obtained by using the right inequality in (3.2). $\square$

Theorem 9. *Let G be an acyclic graph of order n. Then*

$$\begin{array}{ll} (i) & ESO(G) < \binom{n}{2}n, \\ (ii) & ESO_{red}(G) < \binom{n}{2}(n-2). \end{array}$$

Proof. (i) From (3.3), it follows that

$$ESO(G) < \sum_{\substack{\{u,v\}\subseteq V(G)\\ u\neq v}} (d_u + d_v).$$

Since G is an acyclic graph, for any $\{u,v\} \subseteq V(G)$, it holds $d_u + d_v \leq n$. Thus

$$\sum_{\substack{\{u,v\}\subseteq V(G)\\ u\neq v}} (d_u + d_v) \leq \binom{n}{2}n.$$

This completes the proof of (i). Analogously, the inequality (ii) is obtained by using the right inequality in (3.2). $\square$

Remark 2. The bounds for ESO and ESO_{red} in Theorem 4 are sharp compared to those found elsewhere in this section.

4. Chemical trees with maximum and minimum extended Sombor index

In this section, we find the extremal chemical trees of order n with maximum and minimum ESO index. The class of all chemical trees of order n is denoted by $\mathcal{C}(n)$. The extended Sombor index for a chemical tree T can be written as:

$$ESO(T) = \sum_{1 \le i \le j \le 4} c_{ij} \sqrt{i^2 + j^2}. \tag{4.1}$$

It is well-known that the following relations hold:

$$\sum_{1 \le i \le 4} n_i = n. \tag{4.2}$$

$$\sum_{1 \le i \le 4} i n_i = 2n - 2. \tag{4.3}$$

From (1.2) and (4.2), we have the following relations for a chemical tree T:

$$\left.\begin{aligned}
\frac{n_1}{2}(2n - n_1 - 1) &= c_{11} + c_{12} + c_{13} + c_{14} \\
\frac{n_2}{2}(2n - n_2 - 1) &= c_{12} + c_{22} + c_{23} + c_{24} \\
\frac{n_3}{2}(2n - n_3 - 1) &= c_{13} + c_{23} + c_{33} + c_{34} \\
\frac{n_4}{2}(2n - n_4 - 1) &= c_{14} + c_{24} + c_{34} + c_{44}.
\end{aligned}\right\} \tag{4.4}$$

As a consequence of lower bound of Theorem 1, the path graph has minimum ESO index in $\mathcal{C}(n)$.

4.1. Chemical trees with maximum extended Sombor index

Now, we find the extremal chemical trees of order n with the maximum ESO index in $\mathcal{C}(n)$.

Definition 1. Let $n = 3p + q + 1$, where $p \ge 0$ and $1 \le q \le 3$ are both integers. We define

$$\mathcal{D}(n) = \underbrace{4, \ldots, 4}_{p}, q, \underbrace{1, \ldots, 1}_{n-p-1}.$$

Then $\mathcal{D}(n)$ is a sequence of length n. Let $\mathcal{C}(n, p, q) \subseteq \mathcal{C}(n)$ be the set of those chemical trees whose degree sequence in $\mathcal{C}(n)$ is $\mathcal{D}(n)$.

For each $2 \le n \le 3$, we have only one chemical tree in $\mathcal{C}(n)$. Therefore, we only discuss the problem for $n \ge 4$. To find the chemical trees with the maximum extended Sombor index, we need the following lemmas:

Lemma 7. *Let T be a chemical tree in $\mathcal{C}(n)$ of order $n \geq 4$, with the maximum ESO index. Then $n_2(T) \leq 1$.*

Proof. On the contrary, assume that $T \in \mathcal{C}(n)$ has a maximum ESO index with $n_2 > 1$. Let u_1 and v_1 be any two vertices in T, each having a degree 2, and T has a degree sequence

$$(\underbrace{4,\ldots,4}_{p}, \underbrace{3,\ldots,3}_{q}, \underbrace{2,\ldots,2}_{r}, d_{u_1}(T)=2,\, d_{v_1}(T)=2,\, \underbrace{1,\ldots,1}_{n-p-q-r-2}),$$

where $p, q, r \geq 0$. Let v_2 be the other neighbor of v_1 that is not on u_1, v_1-path. We construct a tree $T^* \in C(n)$ from T as follows: $T^* = T - v_1v_2 + v_2u_1$. Then $d_{u_1}(T^*) = d_{u_1}(T) + 1 = 3$, $d_{v_1}(T^*) = d_{v_1}(T) - 1 = 1$ and $d_v(T)$ $=d_v(T^*)$ for all $v \in V(T)\backslash\{u_1,\, v_1\}$. We obtain

$$\begin{aligned}
ESO(T^*) - ESO(T) &= \sqrt{10} - \sqrt{8} + p(\sqrt{25} + \sqrt{17}) + q(\sqrt{18} + \sqrt{10}) + r(\sqrt{13} + \sqrt{5}) \\
&\quad + (n-p-q-r-2)(\sqrt{10} + \sqrt{2}) - p(\sqrt{20} + \sqrt{20}) - q(\sqrt{13} + \sqrt{13}) \\
&\quad - r(\sqrt{8} + \sqrt{8}) - (n-p-q-r-2)(\sqrt{5} + \sqrt{5}). \\
&= \sqrt{10} - \sqrt{8} - 2\sqrt{10} - 2\sqrt{2} + 4\sqrt{5} + p(\sqrt{25} + \sqrt{17} - \sqrt{10} - \sqrt{2} \\
&\quad - 2\sqrt{20} + 2\sqrt{5}) + q(\sqrt{18} + \sqrt{10} - \sqrt{10} - \sqrt{2} - 2\sqrt{13} + 2\sqrt{5}) \\
&\quad + r(\sqrt{13} + \sqrt{5} - \sqrt{10} - \sqrt{2} - 2\sqrt{8} + 2\sqrt{5}) + n(\sqrt{10} + \sqrt{2} - 2\sqrt{5}). \\
&= 0.125 + 0.104n + 0.074p + 0.089q + 0.08r > 0.
\end{aligned}$$

This contradicts our assumption that T has a maximum ESO index in $\mathcal{C}(n)$. Therefore, $n_2(T) \leq 1$. $\square$

Lemma 8. *Let T be a chemical tree in $\mathcal{C}(n)$ of order $n \geq 6$, with maximum ESO index. Then $n_3(T) \leq 1$.*

Proof. On the contrary, assume that $T \in \mathcal{C}(n)$ has a maximum ESO index with $n_3 > 1$. Let u_1 and v_1 be any two vertices in T, each having a degree 3, and T has a degree sequence

$$(\underbrace{4,\ldots,4}_{p}, \underbrace{3,\ldots,3}_{q}, d_{u_1}(T)=3,\, d_{v_1}(T)=3,\, \underbrace{2}_{r},\, \underbrace{1,\ldots,1}_{n-p-q-r-2}),$$

where $p,\, q \geq 0$ and $r \in \{0, 1\}$, by Lemma 7. Let v_2 be the other neighbor of v_1 that is not on u_1, v_1-path. We construct a tree $T^* \in C(n)$ from T as follows: $T^* = T - v_1v_2 + v_2u_1$. Then $d_{u_1}(T^*) = d_{u_1}(T) + 1 = 4$, $d_{v_1}(T^*) = d_{v_1}(T) - 1 = 2$ and $d_v(T)$ $=d_v(T^*)$ for all $v \in V(T)\backslash\{u_1,\, v_1\}$. We obtain

$$\begin{aligned}ESO(T^*) - ESO(T) &= \sqrt{20} + p(\sqrt{32}+\sqrt{20}) + q(\sqrt{25}+\sqrt{13}) + r(\sqrt{20}+\sqrt{8})\\ &+ (n-p-q-r-2)(\sqrt{17}+\sqrt{5}) - \sqrt{18} - p(\sqrt{25}+\sqrt{25})\\ &- q(\sqrt{18}+\sqrt{18}) - r(\sqrt{13}+\sqrt{13}) - (n-p-q-r-2)(\sqrt{10}+\sqrt{10}).\\ &= \sqrt{20} - \sqrt{18} - 2\sqrt{17} - 2\sqrt{5} + 4\sqrt{10} + p(\sqrt{32}+\sqrt{20}-\sqrt{17}-\sqrt{5}\\ &- 2\sqrt{25} + 2\sqrt{10}) + q(\sqrt{25}+\sqrt{13}-\sqrt{17}-\sqrt{5}-2\sqrt{18}+2\sqrt{10})\\ &+ r(\sqrt{20}+\sqrt{8}-\sqrt{17}-\sqrt{5}-2\sqrt{13}+2\sqrt{10}) + n(\sqrt{17}+\sqrt{5}-2\sqrt{10})\\ &= 0.160 + 0.034n + 0.094p + 0.085q + 0.054r > 0.\end{aligned}$$

This contradicts our assumption that T has a maximum ESO index in $\mathcal{C}(n)$. Therefore, $n_3(T) \leq 1$. □

Lemma 9. *Let T be a chemical tree in $\mathcal{C}(n)$ of order $n \geq 5$, with maximum ESO index. Then $n_2(T) + n_3(T) \leq 1$.*

Proof. From Lemmas 7 and 8, we have $n_2(T) \leq 1$ and $n_3(T) \leq 1$. On the contrary, assume that $n_2(T) + n_3(T) = 2$. Then there exist vertices u_1 and v_1 in T of degrees 3 and 2, respectively. Let T has a degree sequence

$$(\underbrace{4,\ldots,4}_{p}, d_{u_1}(T) = 3,\ d_{v_1}(T) = 2,\ \underbrace{1,\ldots,1}_{n-p-2}),$$

where $p \geq 0$. Let v_2 be the other neighbor of v_1 that is not on u_1, v_1-path. We construct a tree $T^* \in C(n)$ from T as follows: $T^* = T - v_1v_2 + v_2u_1$. Then $d_{u_1}(T^*) = d_{u_1}(T) + 1 = 4$, $d_{v_1}(T^*) = d_{v_1}(T) - 1 = 1$ and $d_v(T)$ $=d_v(T^*)$ for all $v \in V(T)\backslash\{u_1, v_1\}$. We obtain

$$\begin{aligned}ESO(T^*) - ESO(T) &= \sqrt{17} + p(\sqrt{32}+\sqrt{17}) + (n-p-2)(\sqrt{17}+\sqrt{2}) - p(\sqrt{25}+\sqrt{20})\\ &\quad - \sqrt{13} - (n-p-2)(\sqrt{10}+\sqrt{5})\\ &= \sqrt{17}\sqrt{13} - 2\sqrt{17} - 2\sqrt{2} + 2\sqrt{10} + 2\sqrt{5} + n(\sqrt{17}+\sqrt{2}-\sqrt{10}-\sqrt{5})\\ &+ p(\sqrt{32}+\sqrt{17}-\sqrt{17}-\sqrt{2}-\sqrt{25}-\sqrt{20}+\sqrt{10}+\sqrt{5}).\\ &= 0.239 + 0.138n + 0.168p > 0.\end{aligned}$$

This contradicts our assumption that T has a maximum ESO index in $\mathcal{C}(n)$. Therefore, $n_2(T) + n_3(T) \leq 1$. □

Theorem 10. *Let T be a chemical tree of order n with maximum ESO index in $\mathcal{C}(n)$.*

Then

$$ESO(T) = \begin{cases} (p+1)(2p+1)\sqrt{2} + 2p(p+1)\sqrt{17} + p(p-1)2\sqrt{2} \\ \qquad\qquad\qquad\qquad\qquad\qquad \text{if } q = 1 \text{ and } n \equiv 2 (\bmod 3), \\ \dfrac{(2p+q)(2p+q-1)}{\sqrt{2}} + q(2p+q)\sqrt{1+q^2} + p\sqrt{16+q^2} \\ \quad + p(2p+q)\sqrt{17} + p(p-1)2\sqrt{2} \\ \qquad\qquad\qquad\qquad\qquad\qquad \text{if } q \in \{2,3\} \text{ and } n \equiv (q-2) (\bmod 3), \end{cases}$$

where p and q are defined in Definition 1.

Proof. Let T be a chemical tree in $\mathcal{C}(n)$ with the maximum ESO index. By Lemma 9, this chemical tree T has $n_2(T) + n_3(T) \leq 1$. As T satisfies $n_2(T) + n_3(T) \leq 1$, the degree sequence of T is $\mathcal{D}(n)$. Now we discuss the problem in two cases.

Case 1. If $q = 1$ in $\mathcal{D}(n)$, then $n_2(T) + n_3(T) = 0$ and $n_4(T) = p$. From (4.2) and (4.3), we get $n_1(T) = 2p + 2$. From (4.2), we obtain $n = 3p + 2$, which implies that $n \equiv 2 (\bmod 3)$. From (1.2), we get

$$\left.\begin{aligned} c_{11} &= (p+1)(2p+1), \\ c_{14} &= 2p(p+1), \\ c_{44} &= \frac{p(p-1)}{2}. \end{aligned}\right\} \tag{4.5}$$

By using (4.5) in (4.1), we obtain

$$ESO(T) \;=\; (p+1)(2p+1)\sqrt{2} + 2p(p+1)\sqrt{17} + p(p-1)2\sqrt{2}.$$

Case 2. If $q \in \{2,3\}$ in $\mathcal{D}(n)$, then $n_2(T) + n_3(T) = 1$ and $n_4(T) = p$. From (4.2) and (4.3), we obtain

$$\left.\begin{aligned} n &= n_1(T) + p + 1, \\ 2n - 2 &= n_1(T) + q + 4p. \end{aligned}\right\} \tag{4.6}$$

From (4.6), we obtain $n_1(T) = 2p + q$. From (4.2), we obtain $n = 3p + q + 1 = 3(p+1) + q - 2$, which implies that $n \equiv q - 2 (\bmod 3)$. From (1.2), we get

$$\left.\begin{aligned} c_{11} &= \frac{(2p+q)(2p+q-1)}{2}, \\ c_{1q} &= q(2p+q), \\ c_{4q} &= p, \\ c_{qq} &= 0, \\ c_{14} &= p(2p+q), \\ c_{44} &= \frac{p(p-1)}{2}. \end{aligned}\right\} \tag{4.7}$$

By using (4.7) in (4.1), we obtain

$$ESO(T) = \frac{(2p+q)(2p+q-1)}{\sqrt{2}} + q(2p+q)\sqrt{1+q^2} + p\sqrt{16+q^2} + p(2p+q)\sqrt{17} + p(p-1)2\sqrt{2}.$$

This finishes the proof. □

5. Chemical significance

As topological indices are rooted in mathematical chemistry, it is important to consider their chemical significance alongside mathematical properties. This section examines the extended Sombor indices as molecular descriptors in QSPR analysis. For a new index to be useful [29], it should effectively model at least one molecular property and provide different structural insights, avoiding high correlation with existing indices. Typically, indices with a correlation coefficient (R) ≥ 0.8 are suitable for regression analysis.

Here we consider benzene hydrocarbons (BHs) to examine the predictive potential of extended Sombor indices. The theoretical values of indices are produced by Python code and the experimental properties are compiled from [32]. We find a significant linear relationship between the extended Sombor indices and the properties of benzene hydrocarbons (BHs), namely boiling point (BP), π-electron energy (π-ele), molecular weight (MW), polarizability (PO), molar refractivity (MR), and molar volume (MV), using a linear model.

BHs properties → / **ESO−indices ↓**	MR	$\pi-$ele	MW	PO	BP	MV
ESO	0.928367	0.918350	0.903492	0.928291	0.836089	0.776136
ESO_{red}	0.910827	0.900013	0.883736	0.910636	0.812371	0.749093
ESO_{avg}	0.930631	0.920939	0.906320	0.930440	0.839465	0.781046

Table 1. The correlation coefficients between extended Sombor indices and physicochemical properties (MR, $\pi-$ele, MW, PO, BP, MV) of benzenoid hydrocarbons (BHs).

Table 1 shows that extended Sombor indices are highly correlated with the physico–chemical properties of BHs, especially with the MR, $\pi-$ele, MW, PO, indicating that these indices could be beneficial in the modeling of these properties.

In examining an important property of a topological molecular descriptor—correlations among extended Sombor indices and degree–based topological indices for octane isomers—we expanded the pool of indices (namely, first and second Zagreb indices [17], Randić index [28], Forgotten index [11] and sum-connectivity index [36]) and calculated their correlation coefficients. These results are given in Table 2.

	SO	SO_{red}	M_1	M_2	R	F	X
ESO	0.719404	0.723579	0.723222	0.698062	0.714617	0.707156	0.724140
ESO_{red}	0.752018	0.754711	0.752511	0.711308	0.749949	0.741979	0.756192
ESO_{avg}	0.725806	0.728887	0.728530	0.699920	0.716092	0.716092	0.725688

Table 2. The correlation coefficient of extended Sombor indices with first Zagreb index (M_1), second Zagreb index (M_2), Randić index, Forgotten index (F) and sum-connectivity index (X).

From Table 2, one can see that ESO, ESO_{red}, and ESO_{avg} are poorly linearly correlated with the indices considered. This finding suggests that the extended Sombor indices offer different structural information compared to the indices in Table 2.

6. Conclusion

In this paper, we introduce the extended versions of Sombor indices based on all pairs of vertices. We have made several important observations. First, we observe that when two non-isomorphic graphs have the same degree sequence, their extended Sombor indices are also the same. This observation has significant implications for understanding graph structures. We explore the basic mathematical features of these extended indices, establish upper and lower bounds in terms of some graph parameters. Furthermore, based on the maximum and minimum extended Sombor index, we characterize the extremal chemical trees. We find that the path graph has the minimum ESO index in $\mathcal{C}(n)$. Additionally, $\mathcal{C}(n,p,q) \subseteq \mathcal{C}(n)$ is the set of chemical trees with a maximum ESO index. For $5 \leq n \leq 11$, $\mathcal{C}(n,p,1)$ has a unique chemical tree for each n, while for $n \geq 12$, $\mathcal{C}(n,p,1)$ has more than one chemical tree. Similarly, for $4 \leq n \leq 8$, $\mathcal{C}(n,p,2)$ and $\mathcal{C}(n,p,3)$ have a unique chemical tree for each n, while for $n \geq 9$, $\mathcal{C}(n,p,2)$ and $\mathcal{C}(n,p,3)$ have more than one chemical tree. Moreover, the chemical significance of the extended Sombor indices has been examined using benzenoid hydrocarbons (BHs), which contain the aforesaid structural features. It has been observed that the extended Sombor indices exhibit considerable predictive potential for the π-electron energy (π-ele), molecular weight (MW), polarizability (PO), and molar refractivity (MR) of BHs.
Future work could explore the extremal bounds of the extended Sombor index in graphs, taking into account additional graph parameters such as the pendant number, branching number, segments, matching, and other related metrics.

Acknowledgements: We would like to gratefully thank the anonymous referee for his invaluable comments and suggestions.

Conflict of Interest: The authors declare no conflict of interest and have received no financial support for this research.

Data Availability: Data sharing is not applicable to this article as no data sets were generated or analyzed during the current study.

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