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Research Article

On higher-order Sombor index

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Abstract: Based on the geometric background of Sombor index and motivating by the higher order connectivity index and the Sombor index, we introduce the path-coordinate of a path in a graph and a degree-point in a higher dimensional coordinate system, and define the higher order Sombor index of a graph. We first consider mathematical properties of the higher order Sombor index, show that the higher order connectivity index of a starlike tree is completely determined by its branches and that starlike trees with a given maximum degree which have the same higher order Sombor indices are isomorphic. Then, we determine the extremal values of the second order Sombor index for all trees with n vertices and characterize the corresponding extremal trees. Finally, the chemical importance of the second order Sombor index is investigated and it is shown that the new index is useful in predicting physicochemical properties with high accuracy compared to some well-established indices.

Keywords: the higher order Sombor index, tree, degree, extremal value

AMS Subject classification: 05C09, 05C90, 05C05, 05C07

1. Introduction

A topological index is a numeric quantity that is mathematically derived in a direct and unambiguous manner from the structural graph of a molecule. Since isomorphic graphs possess identical values for any given topological index, these indices are referred to as graph invariants. Topological indices usually reflect both molecular size and shape. Many topological indices have been developed through the years and correlated with many physical and chemical properties of organic molecules.

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In 1975, Randić [19] introduced the connectivity index (now called also Randić index) as

$$^{1}\chi(G)=\sum_{uv}\frac{1}{\sqrt{d(u)d(v)}} \tag{1}$$

where uv runs over all edges of a graph G and $d(u)$ denotes the degree of vertex u. This index has been successfully related branching in molecular species and become one of the most widely used in applications to physical and chemical properties.
For an integer $h\geq 0$, the connectivity index of order h is defined as

$$^{h}\chi(G)=\sum_{u_1\ldots u_{h+1}}\frac{1}{\sqrt{d(u_1)\ldots d(u_{h+1})}} \tag{2}$$

where $u_1\ldots u_{h+1}$ runs over all paths of length h in G.
The higher order connectivity indices are of great interest in the theory of molecular graph theory ([15, 23]) and some of its mathematical properties have been reported in [3, 17].
In 2021, Gutman [9] introduced the degree-coordinate $(d(u),d(v))$ of an edge uv of a graph G and a degree-point in a two-dimensional coordinate system, and defined the Sombor index of G as the summation of all distances between the degree-points of the edges and the origin over all edges of the graph G, i.e.,

$$SO(G)=\sum_{uv}\sqrt{d(u)^2+d(v)^2} \tag{3}$$

where uv runs over all edges of a graph G. The Sombor index was actually conceived by using the above geometric considerations and attracted much attention, and its numerous mathematical and chemical applications have been established [1, 2, 4–8, 10, 12–14, 16, 18, 20–22]. Geometry-based reasonings reveal the geometric background of several classical topological indices and lead to a series of new SO-like degree-based graph invariants [11].

Motivating by the higher order connectivity index and the Sombor index, we introduce the path-coordinate $(d(u_1),\ldots,d(u_{h+1}))$ of a path $u_1\ldots u_{h+1}$ with length h in a graph G and a degree-point in a $(h+1)$-dimensional coordinate system, and defined the Sombor index of order h (for short, h-order Sombor index) as the summation of the distances between the degree-points and the origin in a $(h+1)$-dimensional coordinate system over all paths with length h in G, i.e.,

$$^{h}SO(G)=\sum_{u_1\ldots u_{h+1}}\sqrt{d(u_1)^2+\cdots+d(u_{h+1})^2} \tag{4}$$

where $u_1\ldots u_{h+1}$ runs over all paths of length h in G. Specifically, $^{0}SO(G)=\sum_{u\in V(G)}d(u)=2|E(G)|$ and the 1-order Sombor index $^{1}SO(G)=\sum_{uv\in E(G)}\sqrt{d(u)^2+d(v)^2}=SO(G)$ is just the Sombor index of G.
In this paper, we first consider mathematical properties of the higher order Sombor indices, show that for every integer $h\geq 0$, the higher order Sombor index $^{h}SO(T)$ of a starlike tree T is completely determined by its branches of length at most h,

and that starlike trees which have equal h-order Sombor index for all $h \geq 0$ are isomorphic. Then, we determine the extremal values of the second order Sombor index for all trees with n vertices and characterize the corresponding extremal trees. Finally, the chemical importance of the second order Sombor index is investigated and it is shown that the new index is useful in predicting physicochemical properties with high accuracy compared to some well-established.

2. Higher order Sombor index of starlike trees

In this section, we first determine the higher order Sombor indices of starlike trees.
Let T be a tree with the maximal degree $\Delta(T)$ and by $k_i(T)$ the number of vertices with degree i. For an integer $m > 2$, a starlike tree T is defined as a tree for which $k_1(T) = \Delta(T) = m$. The set of all starlike trees on n vertices is denoted by Ω_n and the set of all starlike trees on n vertices in which there is a vertex of degree $m > 2$ is denoted by $\Omega_{n,m}$.
For any two vertices u, v in a tree T, we denote by $[u, v]$ the shortest path connecting u and v and the number of edges in $[u, v]$ is the distance in T between u and v, denoted by $d(u, v)$.
If $\{v_1, \cdots, v_m\}$ is the set of vertices with degree 1 and v_0 is the vertex with degree $m > 2$ in $T \in \Omega_{n,m}$ (see Figure 1), an l-branch of T is a subtree $[v_0, v_i]$ in T such that $d(v_0, v_i) = l$. We denote by $S_l(T)$ the number of l-branches in T. Then we have the following "reduction formulas":

$$S_1 + S_2 + \cdots + S_t = m$$

$$S_1 + 2S_2 + \cdots + tS_t = n - 1$$

where t represents the length of the largest branch in T (see Figure 2).

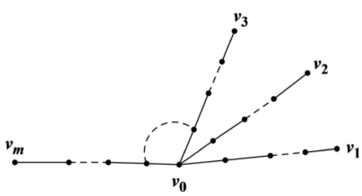

Figure 1. **A starlike tree**

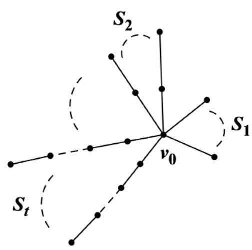

Figure 2. The branches with various lengths

In the following, we will show that the h-order Sombor indices of trees in $\Omega_{n,m}$ are completely determined by the values of $h, n, m, S_1, \cdots, S_h$.
Let $\mathcal{P}_h$ denote the set of all paths of T with length h, $\mathbb{N} = \{0, 1, \cdots\}$ the set of natural numbers and the function $\varphi : \mathcal{P}_h \rightarrow \mathbb{N}^{h+1}$ by $\varphi(v_1 v_2 \cdots v_{h+1}) =$

$(d(v_1), d(v_2), \cdots, d(v_{h+1}))$. Let v_0 be the vertex with degree m of $T \in \Omega_{n,m}$. First, we consider all paths in $\mathcal{P}_h$ not containing v_0 or v_0 is an end vertex. There are only four possibilities $(h+1)$-dimensional vectors for the images under φ of these paths:

$$X_1 = (1, \underbrace{2, \cdots, 2}_{h-1}, m), \quad X_2 = (\underbrace{2, \cdots, 2}_{h}, m), \quad X_3 = (\underbrace{2, \cdots, 2}_{h+1}), \quad X_4 = (1, \underbrace{2, \cdots, 2}_{h}).$$

Next, we consider all paths in $\mathcal{P}_h$ containing v_0 but not as an end vertex of the path. In this case the image of φ maybe as follows:

$Y_1(t) = (1, \underbrace{2, \cdots, 2}_{t}, m, \underbrace{2, \cdots, 2}_{h-t-1})$, where $0 \le t \le h-2$;

$Y_2(t) = (1, \underbrace{2, \cdots, 2}_{t}, m, \underbrace{2, \cdots, 2}_{h-t-2}, 1)$, where $0 \le t \le \lfloor \frac{h}{2} \rfloor - 1$;

$Y_3(t) = (\underbrace{2, \cdots, 2}_{t}, m, \underbrace{2, \cdots, 2}_{h-t})$, where $1 \le t \le \lfloor \frac{h}{2} \rfloor$.

Theorem 1. *Let $T \in \Omega_{n,m}$. Then*

$${}^{h}SO(T) = \lambda(h, n, m, S_1, \cdots, S_{h-1}) + \mu(h, m) S_h$$

where $\lambda(h, n, m, S_1, \cdots, S_{h-1})$ is a real number determined by the values of $h, n, m, S_1, \cdots, S_{h-1}$ and $\mu(h, m) = \sqrt{m^2+4h-3} - \sqrt{m^2+4h} + \sqrt{4h+4} - \sqrt{4h+1} > 0$ is a real number determined by h and m.

Proof. By the definition of h-order Sombor index, ${}^{h}SO(T)$ is determined by $|\varphi^{-1}(X_i)|$ and $|\varphi^{-1}(Y_i(t))|$ which represent the numbers of elements in the inverse image of X_i and Y_i under φ, respectively. In fact,

$$\begin{aligned} {}^{h}SO(T) = & |\varphi^{-1}(X_1)|\sqrt{m^2+4h-3} + |\varphi^{-1}(X_2)|\sqrt{m^2+4h} + |\varphi^{-1}(X_3)|\sqrt{4h+4} \\ & + |\varphi^{-1}(X_4)|\sqrt{4h+1} + \sum_{t=0}^{h-2} |\varphi^{-1}(Y_1(t))|\sqrt{m^2+4h-3} \\ & + \sum_{t=0}^{\lfloor \frac{h}{2} \rfloor - 1} |\varphi^{-1}(Y_2(t))|\sqrt{m^2+4h-6} + \sum_{t=1}^{\lfloor \frac{h}{2} \rfloor} |\varphi^{-1}(Y_3(t))|\sqrt{m^2+4h}. \end{aligned}$$

We can express $|\varphi^{-1}(X_i)|$ and $|\varphi^{-1}(Y_i(t))|$ in terms of $S_1, \cdots, S_h$ by counting argument together with the reduction formulas:

$|\varphi^{-1}(X_1)| = S_h$;

$|\varphi^{-1}(X_2)| = S_{h+1} + \cdots + S_t = m - \sum_{i=1}^{h} S_i$;

$$\begin{aligned} |\varphi^{-1}(X_3)| &= S_{h+2} + 2S_{h+3} + 3S_{h+4} + \cdots + (t-h-1)S_t \\ &= -(h+1)(m - \sum_{i=1}^{h} S_i) + n - 1 - \sum_{i=1}^{h} iS_i; \end{aligned}$$

$|\varphi^{-1}(X_4)| = m - \sum\limits_{i=1}^{h} S_i$;

$$|\varphi^{-1}(Y_1(t))| = \begin{cases} S_{t+1}(m - \sum\limits_{i=1}^{h-t-1} S_i), & 0 \le t \le \frac{h}{2} - 1 \text{ and } h \text{ is even}, \\ S_{t+1}(m - 1 - \sum\limits_{i=1}^{h-t-1} S_i), & \frac{h}{2} \le t \le h-2 \text{ and } h \text{ is even}, \\ S_{t+1}(m - \sum\limits_{i=1}^{h-t-1} S_i), & 0 \le t < \frac{h-1}{2} \text{ and } h \text{ is odd}, \\ S_{t+1}(m - 1 - \sum\limits_{i=1}^{h-t-1} S_i), & \frac{h-1}{2} \le t \le h-2 \text{ and } h \text{ is odd}; \end{cases}$$

$$|\varphi^{-1}(Y_2(t))| = \begin{cases} S_{t+1}S_{h-t-1}, & 0 \le t \le \frac{h}{2} - 2 \text{ and } h \text{ is even}, \\ \frac{1}{2}(S_{t+1} - 1)S_{t+1}, & t = \frac{h}{2} - 1 \text{ and } h \text{ is even}, \\ S_{t+1}S_{h-t-1}, & 0 \le t \le \frac{h-1}{2} - 1 \text{ and } h \text{ is odd}; \end{cases}$$

$$|\varphi^{-1}(Y_3(t))| = \begin{cases} (m - \sum\limits_{i=1}^{h-t} S_i)(m - 1 - \sum\limits_{i=1}^{t} S_i), & 1 \le t \le \frac{h}{2} - 1 \text{ and } h \text{ is even}, \\ \frac{1}{2}(m - \sum\limits_{i=1}^{t} S_i)(m - 1 - \sum\limits_{i=1}^{t} S_i), & t = \frac{h}{2} \text{ and } h \text{ is even}, \\ (m - \sum\limits_{i=1}^{h-t} S_i)(m - 1 - \sum\limits_{i=1}^{t} S_i), & 1 \le t \le \frac{h-1}{2} \text{ and } h \text{ is odd}. \end{cases}$$

It can be seen from above that for all t, $|\varphi^{-1}(Y_i(t))|$ $(i = 1, 2, 3)$ depends on the numbers $h, m, S_1, \cdots, S_{h-1}$ while $|\varphi^{-1}(X_i)|$ $(i = 1, 2, 3, 4)$ depends on the numbers $h, m, S_1, \cdots, S_h$. By grouping appropriately, we obtain

$$^{h}SO(T) = \lambda(h, n, m, S_1, \cdots, S_{h-1}) + \mu(h, m)S_h$$

where $\lambda(h, n, m, S_1, \cdots, S_{h-1})$ is a real number determined by the values of $h, n, m, S_1, \ldots, S_{h-1}$ and $\mu(h, m) = \sqrt{m^2 + 4h - 3} - \sqrt{m^2 + 4h} + \sqrt{4h + 4} - \sqrt{4h + 1} > 0$ is a real number determined by h and m. □

As $\lambda(h, n, m, S_1, \cdots, S_{h-1})$ is determined by $h, n, m, S_1, \cdots, S_{h-1}$ and $\mu(h, m) > 0$ is determined by h and m, we can get from Theorem 1.

Corollary 1. *Let $T, T' \in \Omega_{n,m}$. If $S_i(T) = S_i(T')$ for all $i = 1, \cdots, h - 1$, then $^{h-1}SO(T) = {}^{h-1}SO(T')$. Moreover, $^{h}SO(T) > {}^{h}SO(T') \Leftrightarrow S_h(T) > S_h(T')$.*

Also, Theorem 1 shows that for a $T \in \Omega_{n,m}$, only the l-branches $(l \le h)$ in T contribute to $^{h}SO(T)$. This fact is crucial in the following result, which shows that a starlike tree with a given maximum degree is completely determined by its higher-order Sombor indices.

Corollary 2. *Let $T \in \Omega_{n,m}$ and $T' \in \Omega_{n',m}$. Then T and T' are isomorphic if and only if $^{h}SO(T) = {}^{h}SO(T')$ for all $h \ge 0$.*

Proof. If T and T' are isomorphic, then it is clear that $^{h}SO(T) = {}^{h}SO(T')$ for all $h \ge 0$.
Conversely, assume that $T \in \Omega_{n,m}$ and $T' \in \Omega_{n',m}$. Since $^{0}SO(T) = 2|E(T)| = {}^{0}SO(T') = 2|E(T')|$, $n = n'$. Now, applying Theorem 1 for $h = 1$, we get $\lambda(1, n, m) +$

$\mu(1,m)S_1(T) = \lambda(1,n,m) + \mu(1,m)S_1(T')$. And $S_1(T) = S_1(T')$ for $\mu(1,m) \neq 0$. Assume that $S_i(T) = S_i(T')$ for all $i = 1, \cdots, h-1$, by Theorem 1 again, we can conclude $S_h(T) = S_h(T')$. By induction, we have that $S_i(T) = S_i(T')$ for all $i \geq 1$. So, T and T' are isomorphic. □

We guess that all starlike tress are completely characterized by their higher-order Sombor indices.

Conjecture 2. Let T, T' be starlike trees. Then T and T' are isomorphic if and only if ${}^hSO(T) = {}^hSO(T')$ for all $h \geq 0$.

3. The extremal values of second order Sombor indices for trees

In this section, we consider the second order Sombor index of trees.
If $P = uu_1u_2 \ldots u_k$ is a path of length k in a graph G such that $d(u) \geq 3$, $d(u_k) = 1$ and $d(u_i) = 2$ for $i = 1, 2, \cdots, k-1$, then P is called a pendent path of G, u and k are the origin and the length of P, respectively.

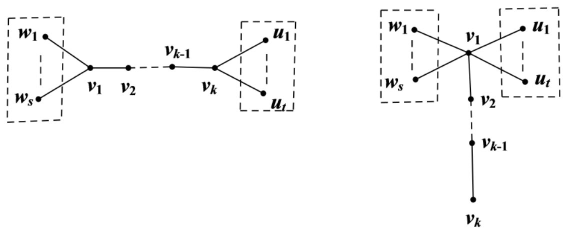

Figure 3. **path-lifting transformation**

Lemma 1. *(Path-lifting transformation) Let $P = v_1v_2 \cdots v_k$ be an induced path in a graph G, where $d(v_1), d(v_k) \geq 2$ and $d(v_i) = 2$, $i = 2, \cdots, k-1$. $G' = G - \{v_kw : w \in N(v_k) \setminus \{v_{k-1}\}\} + \{v_1w : w \in N(v_k) \setminus \{v_{k-1}\}\}$ (see Figure 3), then ${}^2SO(G) < {}^2SO(G')$.*

Proof. Let $N_G(v_1) = \{v_2, w_1, \ldots w_s\}$, $N_G(v_k) = \{v_{k-1}, u_1, \ \ldots, \ u_t\}$, $s, t \geq 1$; $N_G(w_i) = \{v_1, w_{i1}, \ \ldots, \ w_{ik_i}\}$, $N_{G'}(w_i) = \{v_1, w_{i1}, \ \ldots, \ w_{ik_i}\}$, where $i = 1, \ldots, s$, $k_i \geq 0$; $N_G(u_j) = \{v_k, u_{j1}, \ldots, \ u_{jg_j}\}$, $N_{G'}(u_j) = \{v_1, u_{j1}, \ldots, \ u_{jg_j}\}$, where $j = 1, \ldots, t$, $g_j \geq 0$; $N_{G'}(v_1) = \{v_2, w_1, \ldots w_s, u_1, \cdots, u_t\}$. Only the degrees of v_1 and v_k have changed in the transformation. Consider the paths of length 2 in G which contain v_1 or v_k, there are the following possibilities:
$A_i = \{w_{i_j}w_iv_1 | 0 \leq j \leq k_i\}$, $A = A_1 \cup \cdots \cup A_s$;
$B_i = \{u_{i_j}u_iv_k | 0 \leq j \leq g_i\}$, $B = B_1 \cup \cdots \cup B_t$;
$C = \{w_iv_1w_j | 1 \leq i < j \leq s\}$, $D = \{u_iv_ku_j | 1 \leq i < j \leq t\}$;

$M = \{w_i v_1 v_2, u_j v_k v_{k-1} | 1 \le i \le s, 1 \le j \le t\}$;

$L = \begin{cases} \{v_1 v_2 v_3, v_{k-2} v_{k-1} v_k\}, & k \ge 3 \\ \emptyset, & k = 2 \end{cases}$.

Also, there are only the following possibilities for the paths of length 2 containing v_1 or v_k in G':

$A'_i = \{w_{i_j} w_i v_1 | 0 \le j \le k_i\}$, $A' = A'_1 \cup \cdots \cup A'_s$;

$B'_i = \{u_{i_j} u_i v_1 | 0 \le j \le g_i\}$, $B' = B'_1 \cup \cdots \cup B'_t$;

$C' = \{w_i v_1 w_j | 1 \le i < j \le s\}$, $D' = \{u_i v_1 u_j | 1 \le i < j \le t\}$;

$M' = \{w_i v_1 u_j, w_i v_1 v_2, u_j v_1 v_2 | 1 \le i \le s, 1 \le j \le t\}$;

$L' = \begin{cases} \{v_1 v_2 v_3, v_k v_{k-1} v_{k-2}\} & k \ge 3 \\ \emptyset, & k = 2 \end{cases}$

Then

$$\begin{aligned}
&{}^2SO(G') - {}^2SO(G) \\
&= \sum_{xyz \in A'} \sqrt{d(x)^2 + d(y)^2 + d(z)^2} - \sum_{xyz \in A} \sqrt{d(x)^2 + d(y)^2 + d(z)^2} \\
&+ \sum_{xyz \in B'} \sqrt{d(x)^2 + d(y)^2 + d(z)^2} - \sum_{xyz \in B} \sqrt{d(x)^2 + d(y)^2 + d(z)^2} \\
&+ \sum_{xyz \in C'} \sqrt{d(x)^2 + d(y)^2 + d(z)^2} - \sum_{xyz \in C} \sqrt{d(x)^2 + d(y)^2 + d(z)^2} \\
&+ \sum_{xyz \in D'} \sqrt{d(x)^2 + d(y)^2 + d(z)^2} - \sum_{xyz \in D} \sqrt{d(x)^2 + d(y)^2 + d(z)^2} \\
&+ \sum_{xyz \in M'} \sqrt{d(x)^2 + d(y)^2 + d(z)^2} - \sum_{xyz \in M} \sqrt{d(x)^2 + d(y)^2 + d(z)^2} \\
&+ \sum_{xyz \in L'} \sqrt{d(x)^2 + d(y)^2 + d(z)^2} - \sum_{xyz \in L} \sqrt{d(x)^2 + d(y)^2 + d(z)^2} \\
&= S_1 + S_2 + S_3 + S_4 + S_5 + S_6
\end{aligned}$$

where

$$\begin{aligned}
S_1 &= \sum_{xyz \in A'} \sqrt{d(x)^2 + d(y)^2 + d(z)^2} - \sum_{xyz \in A} \sqrt{d(x)^2 + d(y)^2 + d(z)^2} \\
&= \sum_{i=1}^{s} \sum_{j=1}^{k_i} \left(\sqrt{d(w_{ij})^2 + d(w_i)^2 + (s+t+1)^2} - \sqrt{d(w_{ij})^2 + d(w_i)^2 + (s+1)^2} \right) \\
&\ge 0
\end{aligned}$$

$$S_2 = \sum_{xyz \in B'} \sqrt{d(x)^2 + d(y)^2 + d(z)^2} - \sum_{xyz \in B} \sqrt{d(x)^2 + d(y)^2 + d(z)^2} \ge 0$$

$$\begin{aligned}
S_3 &= \sum_{xyz \in C'} \sqrt{d(x)^2 + d(y)^2 + d(z)^2} - \sum_{xyz \in C} \sqrt{d(x)^2 + d(y)^2 + d(z)^2} \\
&= \sum_{i=1}^{s-1} \sum_{j=i+1}^{s} \left(\sqrt{d(w_j)^2 + d(w_i)^2 + (s+t+1)^2} - \sqrt{d(w_j)^2 + d(w_i)^2 + (s+1)^2} \right) \\
&\ge 0
\end{aligned}$$

$$S_4 = \sum_{xyz\in D'} \sqrt{d(x)^2+d(y)^2+d(z)^2} - \sum_{xyz\in D} \sqrt{d(x)^2+d(y)^2+d(z)^2} \geq 0$$

$$\begin{aligned} S_5 &= \sum_{xyz\in M'} \sqrt{d(x)^2+d(y)^2+d(z)^2} - \sum_{xyz\in M} \sqrt{d(x)^2+d(y)^2+d(z)^2} \\ &= \sum_{i=1}^{s} \left(\sqrt{(s+t+1)^2+d(w_i)^2+d_{G'}(v_2)^2} - \sqrt{(s+1)^2+d(w_i)^2+d_G(v_2)^2} \right) \\ &\quad + \sum_{j=1}^{t} \left(\sqrt{(s+t+1)^2+d(u_j)^2+d_{G'}(v_2)^2} - \sqrt{(t+1)^2++d(u_j)^2+d_G(v_{k-1})^2} \right) \\ &\quad + \sum_{i=1}^{s}\sum_{j=1}^{t} \sqrt{d(w_i)^2+(s+t+1)^2+d(u_j)^2} \\ &> 0 \end{aligned}$$

$$S_6 = \sum_{xyz\in L'} \sqrt{d(x)^2+d(y)^2+d(z)^2} - \sum_{xyz\in L} \sqrt{d(x)^2+d(y)^2+d(z)^2}$$

and $S_6 = 0$ when $k = 2$, $S_6 = \sqrt{(s+t+1)^2+5} - \sqrt{(t+1)^2+(s+1)^2+4} > 0$ when $k = 3$, $S_6 = \sqrt{(s+t+1)^2+8}+3-\sqrt{(t+1)^2+8}-\sqrt{(s+1)^2+8} > 0$ when $k > 3$. So, we have ${}^2SO(G) < {}^2SO(G')$. □

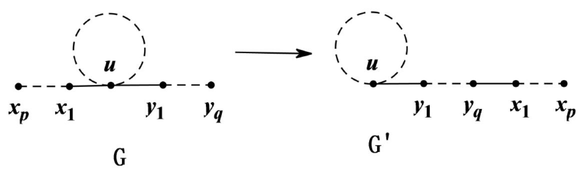

Figure 4. **sliding transformation**

The sliding transformation in the following is a special case of the path-lifting transformation (Lemma 1) in a reverse direction.

Lemma 2. *(Sliding transformation) Let $P = ux_1 \ldots x_p$ and $Q = uy_1 \ldots y_q$ be two pendant paths with origins u, where $d(u) > 2$ and $1 \leq p \leq q$, $G' = G - \{ux_1\} + \{x_1y_q\}$ (see Figure 4). Then ${}^2SO(G') < {}^2SO(G)$.*

Proof. It can be directly obtained from Lemma 1 by lifting the path $P = uy_1 \cdots y_q$ in G'. □

The following result shows that the tree with the minimum 2-order Sombor index is P_n and the tree with the maximum 2-order Sombor index is S_n among all trees with n vertices.

Theorem 3. *Let T be a tree with $n \geq 4$ vertices, then*

$$6 + 2(n-4)\sqrt{3} \leq {}^2SO(T) \leq \binom{n-1}{2}\sqrt{2+(n-1)^2}$$

with left equality if and only if $T \cong P_n$ and right equality if and only if $T \cong S_n$.

Proof. It is well known that any tree T with n vertices can be transformed into the star S_n by repeated use of the path-lifting transformation (Lemma 1), we have

$${}^2SO(T_n) \leq {}^2SO(S_n) = \binom{n-1}{2}\sqrt{2+(n-1)^2}$$

with equality if and only if $T \cong S_n$.
Similarly, a tree T with n vertices can be transformed into the path P_n by using sliding-transformation in Lemma 2, we have

$${}^2SO(T_n) \geq {}^2SO(P_n) = 6 + 2(n-4)\sqrt{3}$$

with equality if and only if $T \cong P_n$. □

Next, we discuss the extremal values of 2-order Sombor index for all trees with n vertices and the maximum degree Δ.
Denote by $\mathcal{T}_n^{\Delta}$ the set of all trees with n vertices and the maximum degree Δ.
Let $T \in \mathcal{T}_n^{\Delta}$. Using path-lifting transformation repeatedly on the outermost branch vertices (keeping one vertex with the maximum degree) in T, we can get a starlike tree T'. By Lemma 2, ${}^2SO(T) \geq {}^2SO(T')$. So, the tree in $\mathcal{T}_n^{\Delta}$ with the minimum 2-order Sombor index is a starlike tree in $\Omega_{n,m}$, where $m = \Delta$.
Now, we characterize the extremal tree with the minimum second order Sombor index in $\Omega_{n,m}$.

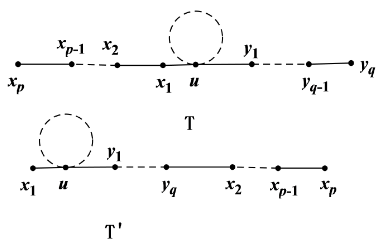

Figure 5. **The graphs in Lemma 3**

Lemma 3. *Let $P = ux_1 \dots x_p$ and $Q = uy_1y_2 \dots y_q$ be two pendant paths with the origin u in a tree T, where $p, q \geq 2$, and $T' = T - \{x_1x_2\} + \{y_qx_2\}$, see Figure 5, then* ${}^2SO(T') < {}^2SO(T)$.

Proof. Let $N_G(u) = \{x_1, u_1, u_2, \dots, u_s\}$, where $u_s = y_1$ and $s \geq 2$. From T to T', only the degrees of x_1 and y_q have changed. Consider the paths of length 2 in T containing x_1 or y_q:
$A = \{u_i u x_1 | 1 \leq i \leq s\}$,

$$B = \begin{cases} \{ux_1x_2, x_1x_2x_3, y_{q-2}y_{q-1}y_q\}, & p \geq 3, q \geq 3 \\ \{ux_1x_2, x_1x_2x_3, uy_1y_2\}, & p \geq 3, q = 2 \\ \{ux_1x_2, y_{q-2}y_{q-1}y_q\}, & p = 2, q \geq 3 \\ \{ux_1x_2, uy_1y_2\}, & p = q = 2 \end{cases}$$

Also, the paths of length 2 in T' containing x_1 or y_q: $A' = \{u_i u x_1 | 1 \leq i \leq s\}$,

$$B' = \begin{cases} \{y_{q-2}y_{q-1}y_q, y_{q-1}y_qx_2, y_qx_2x_3\}, & p \geq 3, q \geq 3 \\ \{uy_1y_2, y_1y_2x_2, y_2x_2x_3\}, & p \geq 3, q = 2 \\ \{y_{q-2}y_{q-1}y_q, y_{q-1}y_qx_2\}, & p = 2, q \geq 3 \\ \{uy_1y_2, y_1y_2x_2\}, & p = q = 2 \end{cases}$$

Then

$$\begin{aligned} & {}^2SO(T) - {}^2SO(T') \\ &= \sum_{xyz \in A} \sqrt{d(x)^2 + d(y)^2 + d(z)^2} - \sum_{xyz \in A'} \sqrt{d(x)^2 + d(y)^2 + d(z)^2} \\ &+ \sum_{xyz \in B} \sqrt{d(x)^2 + d(y)^2 + d(z)^2} - \sum_{xyz \in B'} \sqrt{d(x)^2 + d(y)^2 + d(z)^2} \\ &= S_1 + S_2 \end{aligned}$$

where

$$\begin{aligned} S_1 &= \sum_{xyz \in A} \sqrt{d(x)^2 + d(y)^2 + d(z)^2} - \sum_{xyz \in A'} \sqrt{d(x)^2 + d(y)^2 + d(z)^2} \\ &= \sum_{i=1}^{s} \left(\sqrt{d(u_i)^2 + (s+1)^2 + 4} - \sqrt{d(u_i)^2 + (s+1)^2 + 1} \right) \\ &> 0 \end{aligned}$$

$$S_2 = \sum_{xyz \in B} \sqrt{d(x)^2 + d(y)^2 + d(z)^2} - \sum_{xyz \in B'} \sqrt{d(x)^2 + d(y)^2 + d(z)^2}.$$

When $p \geq 3, q \geq 3$, $S_2 = \sqrt{(s+1)^2 + 8} + 3 - 4\sqrt{3} > 0$;
When $p \geq 3, q = 2$, $S_2 = \sqrt{(s+1)^2 + 5} - 2\sqrt{3} > 0$;
When $p = 2, q \geq 3$, $S_2 = \sqrt{(s+1)^2 + 5} - 2\sqrt{3} > 0$;
When $p = q = 2$,

$$S_2 = \sqrt{(s+1)^2 + 5} + \sqrt{(t+1)^2 + 5} - \sqrt{(t+1)^2 + 8} - 3 > 0.$$

In conclusion, ${}^2SO(T') < {}^2SO(T)$. □

By $S(n_1, \dots, n_m)$, we denote the starlike tree with the center u of degree $m > 2$ such that

$$S(n_1, \dots, n_m) - u = P_{n_1} \cup P_{n_2} \cdots \cup P_{n_m}$$

where $1 \leq n_1 \leq n_2 \cdots \leq n_m$.

Theorem 4. *Let $T \in \Omega_{n,m}$, where $n - m \geq 3$, then*

$$^2SO(T) \geq \frac{(m-1)(m-2)}{2}\sqrt{2+m^2} + (m-1)\sqrt{5+m^2} + \sqrt{m^2+8} + 2(n-m-3)\sqrt{3} + 3$$

with equality if an only if $T \cong S(\underbrace{1,\ldots,1}_{m-1}, n-m)$.

Proof. Let $T \in \Omega_{n,m}$ be a tree with the minimum 2-order Sombor index. If $T \neq S(\underbrace{1,\cdots,1}_{m-1}, n-m)$, then there are two pendant paths $P = vx_1\cdots x_p$ and $Q = vy_1\cdots y_q$ in T with length at least 2, where $d(v) = m$ and $p, q \geq 2$. Let $T' = T - \{x_1x_2\} + \{y_qx_2\}$. Then $T' \in \Omega_{n,m}$ and $^2SO(T') < {}^2SO(T)$ from Lemma 3, a contradiction. □

As we know from above, the tree in $\mathcal{T}_n^{\Delta}$ with the minimum 2-order Sombor index is a starlike tree in $\Omega_{n,\Delta}$. By Theorem 4, we have

Corollary 3. *Let $T \in T_n^{\Delta}$, then*

$$^2SO(T) \geq {}^2SO(S(\underbrace{1,\ldots,1}_{\Delta-1}, n-\Delta))$$

with equality if an only if $T \cong S(\underbrace{1,\ldots,1}_{\Delta-1}, n-\Delta)$.

Further, let

$$\begin{aligned} f(m) &= {}^2SO(S(\underbrace{1,\cdots,1}_{m-1}, n-m)) \\ &= \frac{(m-1)(m-2)}{2}\sqrt{2+m^2} + (m-1)\sqrt{5+m^2} + \sqrt{m^2+8} + 2(n-m-3)\sqrt{3} + 3 \end{aligned}$$

where $2 \leq m \leq n-1$. It is easy to prove that the minimum value of $f(m)$ is $f(2)$. So, the tree with the minimum 2-order Sombor index in Ω_n is P_n. This is consistent with the result in Theorem 3.

In the following, we describe the extremal tree with the maximum 2-order Sombor index in $\Omega_{n,m}$.

Lemma 4. *Let $P = ux_1\cdots x_p$ and $Q = uy_1y_2\cdots y_q$ be two pendant paths with origin u in a tree T, where $p, q \geq 3$, and $T' = T - \{x_2x_3\} + \{y_qx_3\}$, see Figure 6. Then $^2SO(T') > {}^2SO(T)$.*

Proof. It can be seen that

$$^2SO(T') - {}^2SO(T) = \sqrt{5+d(u)^2} + 2\sqrt{3} - \sqrt{8+d(u)^2} - 3 > 0.$$

Thus the conclusion is true. □

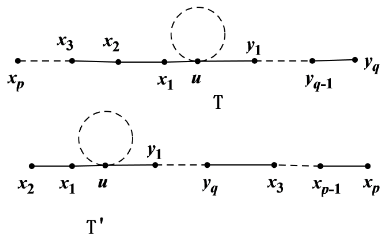

Figure 6. **Trees in Lemma 4**

Theorem 5. *If $n \geq 2m+1$, then the tree with the maximum 2-order Sombor index in $\Omega_{n,m}$ is $S(\underbrace{2,\cdots,2}_{m-1},n+1-2m)$. If $n < 2m+1$, then the tree with the maximum 2-order Sombor index in $\Omega_{n,m}$ is $S(\underbrace{1,\cdots,1}_{2m+1-n},\underbrace{2,\cdots,2}_{n-1-m})$.*

Proof. Let $T \in \Omega_{n,m}$ be a tree with the maximum 2-order Sombor index and v the center with degree m in T.
When $n \geq 2m+1$, T has a pendant path $P = vy_1 \cdots y_q$ with length at least 3 if $S_1(T) \neq 0$, where $q \geq 3$. Let $T' = T - \{y_{q-1}y_q\} + \{xy_q\}$, we have ${}^2SO(T') > {}^2SO(T)$ from Lemma 3, a contradiction. So, $S_1(T) = 0$. If $S_2(T) \leq m-1$, then T has two pendent paths $P = vx_1 \cdots v_p$ and $Q = vy_1 \cdots y_q$ with length at least 3, where $p, q \geq 3$. Let $T'' = T - \{x_2x_3\} + \{y_qx_3\}$, we have ${}^2SO(T'') > {}^2SO(T)$ from Lemma 4, a contradiction. So, $T \cong S(\underbrace{2,\ldots,2}_{m-1},n+1-2m)$.
When $n < 2m+1$, T must have a pendant edge vx. If T has a pendant path $P = vx_1 \cdots x_p$ with length at least 3, let $T''' = T - \{x_{p-1}x_p\} + \{xx_p\}$, then we have ${}^2SO(T''') > {}^2SO(T)$ by Lemma 3, a contradiction. So, $T \cong S(\underbrace{1,\ldots,1}_{2m+1-n},\underbrace{2,\ldots,2}_{n-1-m})$ and the proof is completed. □

4. The chemical application of second order Somber index

In this section, the chemical applicability of the second order Somber index is studied. Usually, octane isomers are helpful for such investigation, since they represent a sufficiently large and structurally diverse group of alkane for the preliminary testing of indices. In order to investigate predictive capability of the second order Sombor index, we establish the applicability of the second order Sombor index for octane isomer, and develop models for predicting the entropy (S) and AcenFac of octane isomers were developed. The experimental date used for the construction of the models was collected from *http : //www.moleculardescriptors.eu/dataset/dataset.htm* and they are presented in Table 4 (columns 2-3).

The initial step for developing a linear model for predicting the AcenFac of molecules was to correlate the calculated values of the second order Sombor index and the Sombor index (column 3-4 of Table 4) with the experimental date of octane isomers. With this, it was checked whether the second order Sombor index and the Sombor index contain information that may be used to model AcenFac. The AcenFac values are plotted in Figure 7, which shows a reasonable correlation between the second order Sombor index and AcenFac. Such a correlation indicates that a linear model for predicting the AcenFac of octane isomers could be developed using the second order Sombor index. The correlations between Sombor index and AcenFac are depicted in Figure 8. Since the second order Sombor index shows satisfactory correlation with

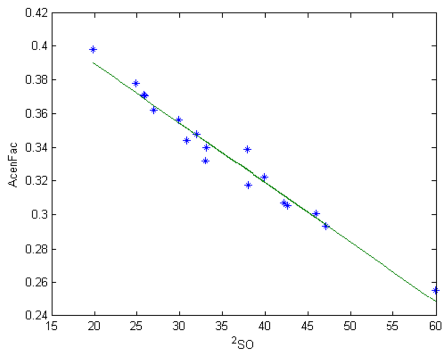

Figure 7. **AcentFac and ^2SO**

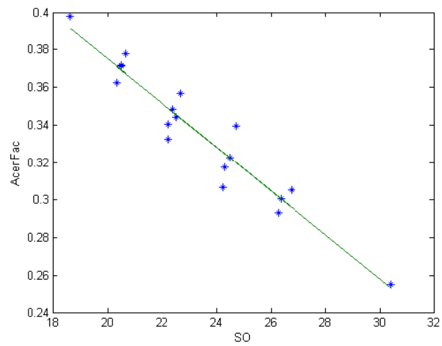

Figure 8. **AcentFacd and SO**

the AcenFac of octane isomers, the correlation between second order Sombor index and the entropy (S) of octane isomers was tested Table 1 (column 2). The correlation between the second order Sombor index and entropy (S) is depicted in Figure 9. The scatter plot presented in Figure 9 shows that a linear dependence between the second order Sombor index and entropy. The correlations between Sombor index and is entropy (S) depicted in Figure **??**.

As all examined correlations show linear relationships between the second order Sombor index and these two physico-chemical properties, a linear model was constructed in (5).

$$AcenFac, S \approx A \times TI + B \tag{5}$$

where TI stands for the ^2SO and SO, where A and B is the fitting coefficient. The values for the parameters are presented in Table 2.

Correlations of the second order Sombor index ^2SO with AcenFac and entropy are shown in Table 3. The correlation coefficients of ^2SO for octane isomers are 0.9849 and 0.9618 with AcenFac and entropy, stronger than that of the Sombor index SO. The index ^2SO shows better predictive capability than the Sombor index for AcenFac and entropy. These results confirm the suitability of ^2SO in QSPR analysis.

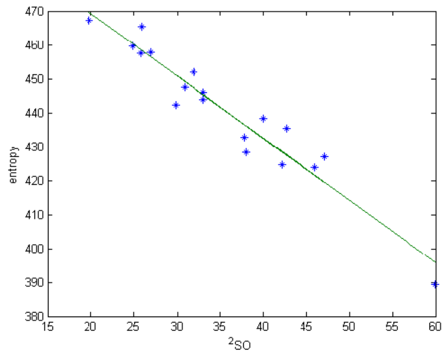

Figure 9. entropy and ^2SO

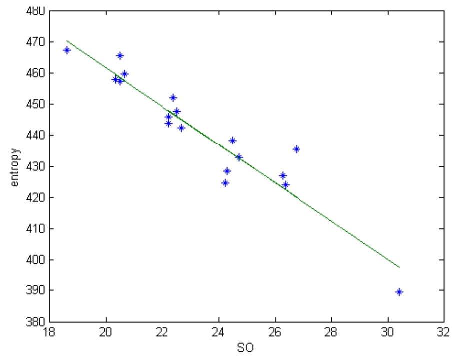

Figure 10. entropy and SO

Table 1. Experimental values of the entropy, acentric factor and the corresponding values of degree based topological indices of octane isomer

Alkane	S	AcenFac	^2SO	SO
n-octane	467.23	0.397898	19.8564	18.6143
2-methyl-heptane	459.57	0.377916	24.8512	20.6515
3-methyl-heptane	465.51	0.371002	25.9353	20.5024
4-methyl-heptane	457.39	0.371504	25.8526	20.5024
3-ethyl-hexane	457.86	0.362472	26.9757	20.3532
2,2-dimethyl-hexane	432.71	0.339426	37.8387	24.7344
2,3-dimethyl-hexane	451.96	0.348247	31.9485	22.3995
2,4-dimethyl-hexane	447.60	0.344223	30.8383	22.5396
2,5-dimethyl-hexane	442.33	0.35683	29.8461	22.6886
3,3-dimethyl-hexane	438.23	0.322596	39.9535	24.4910
3,4-dimethyl-hexane	445.97	0.340345	33.0653	22.2504
2-methyl-3-ethyl-pentane	443.76	0.332433	33.0217	22.2504
3-methyl-3-ethyl-pentane	424.59	0.304899	42.1924	24.2477
2,2,3-trimethyl-pentane	423.88	0.300816	45.9925	26.3732
2,2,4-trimethyl-pentane	435.51	0.30537	42.6608	26.7716
2,3,3-trimethyl-pentane	427.02	0.293177	47.0822	26.2790
2,3,4-trimethyl-pentane	428.40	0.317422	37.9928	24.2967
2,2,3,3-tetramethylbutane	389.36	0.255294	59.9232	30.3955

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Conflict of interest. The authors declare that they have no conflict of interest.

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

Table 2. **Correlation coefficient with and residual standard error of regression model**

parameter	TI	A	B
AcenFac	^2SO	-0.003532	0.4605
	SO	-0.005857	0.6093
entropy	^2SO	-1.839	506.1
	SO	-3.081	584.9

Table 3. **Correlation coefficient with and residual standard error of regression model**

parameter	TI	Correlation coefficient(R)	RMSE
AcenFac	^2SO	0.9849	0.006319
	SO	0.9594	0.0103
entropy	^2SO	0.9618	5.335
	SO	0.9465	6.287

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