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Research article

Extremal values of the modified Sombor index in trees

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Abstract: Based on Euclidean metrics, Gutman put forward a novel vertex-degree-based topological index, named the Sombor index. Later, the modified version of it—the modified Sombor index—was introduced. For a simple undirected graph G, the Sombor index and the modified Sombor index of G are defined as $SO(G) = \sum_{uv\in E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}$ and ${}^mSO(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_G(u)^2+d_G(v)^2}}$, respectively, where $d_G(w)$ denotes the degree of w in G. Extremal values of SO have been intensively investigated. In this paper, we were concerned with the extremal values of the modified Sombor indices. First, we showed some graph transformations which can be used to compare the modified Sombor indices of two graphs. With these transformations, the first two maximum and minimum values of ${}^mSO$ among all trees of order n were determined. We also characterized the unique tree that minimizes ${}^mSO$ among all trees with a fixed number of pendant vertices. In addition, the molecular trees with the maximum and minimum modified Sombor indices were investigated.

Keywords: extremal value; Sombor index; modified Sombor index; tree; molecular tree
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1. Introduction

In this paper, only simple, undirected, and connected graphs will be in consideration. Suppose $G = (V(G), E(G))$ is a graph of order n and size m. The complement $\overline{G}$ of G is the simple graph such that $V(\overline{G}) = V(G)$, and $uv \in E(\overline{G})$ iff $uv \notin E(G)$. Let $N_G(v)$ be the set of vertices adjacent to v in G. Then the cardinality of $N_G(v)$, always denoted by $d_G(v)$, is called the degree of v in G. If $d_G(v) = 1$, then v is said to be a pendant vertex or leaf of G. Otherwise, v is a non-pendant vertex of G. Let $\Delta(G)$

be the maximum degree of G. G is a chemical graph or molecular graph if $\Delta(G) \leq 4$. Denote by S_n, P_n, and C_n the star, path, and cycle of order n, respectively. For a path $P = vv_1v_2 \cdots v_r$ in graph G, if $d_G(v) \geq 3$, $d_G(v_r) = 1$, and $d_G(v_i) = 2$ for $1 \leq i \leq r-1$, then P is known as a pendant path of G and v is the origin of P. For a subset $D \subseteq E(G)$ (or $D \subseteq V(G)$), let $G - D$ denote the graph gained from G by deleting every element in D. If $D \subseteq E(\overline{G})$, let $G + D$ be the graph gained from G by adding each element in D to G. For notations and terminologies undefined here, we refer the readers to [1].

Molecules can be considered as molecular graphs where vertices represent atoms, while edges represent the chemical bonds between atoms. One common issue in theoretical chemistry is to correlate molecular structures with biological and physicochemical properties of molecules. To accomplish this, many topological indices (or molecular structure descriptors) have been introduced and studied over the years. A topological index of a graph G is a single number related to G which stays the same under graph isomorphism.

Motivated by Euclidean metrics, a vertex-degree-based topological index, named the Sombor index, was introduced by Gutman [2] recently. It is defined as

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

where $d_G(w)$ denotes the degree of the vertex w in G. Gutman [2] also proposed the reduced Sombor index, defined as

$$SO_{red}(G) = \sum_{uv \in E(G)} \sqrt{(d_G(u)-1)^2 + (d_G(v)-1)^2},$$

and established some basic properties of the Sombor index. The chemical applicability of SO is examined in [3, 4] and this new index shows good predictive potential and suitability in QSPR analysis. The mathematical properties of the Sombor index have also been intensively investigated. For example, in the review [5], Liu et al. collected numerous bounds and extremal results on the Sombor index of graphs in terms of various graph parameters. Some studies [6–8] focused on the graphs such that their Sombor indices are integers. Kulli and Gutman computed Sombor indices of certain networks in [9]. Several extremal results for molecular graphs are derived in [3, 10–13]. Spectral properties of Sombor matrices are also considered in [14–20].

After defining the Sombor index and reduced Sombor index, Kulli and Gutman [9] put forward the modified Sombor index and reduced modified Sombor index, defined as

$$^{m}SO(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u)^2 + d_G(v)^2}},$$

and

$$^{m}SO_{red}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{(d_G(u)-1)^2 + (d_G(v)-1)^2}},$$

respectively. They also gave exact formulas for certain chemical networks in [9]. In [21], Huang and Liu obtained some bounds for the modified Sombor indices of graphs and also some relationships between ^{m}SO and some other indices. Shooshtari et al. [22] gave a sharp lower bound on the modified Sombor index of unicyclic graphs with a fixed diameter. Results concerning the modified Sombor matrix can be found in [21, 23] and the chemical applicability of the modified Sombor index can be seen in [23].

Inspired by numerous extremal results of the Sombor index, it is natural to consider the extremal values of the modified Sombor index in trees. We first show some graph transformations which can be used to compare the modified Sombor indices of two graphs in Section 2. With these transformations, the first two maximum and minimum trees are determined in Section 3. We also characterize the unique tree that minimizes ${}^{m}SO$ among all trees with a fixed number of pendant vertices. In Section 4, the molecular trees with the maximum and minimum modified Sombor indices are investigated.

2. Preliminaries

In this section, we give some transformations that can influence the modified Sombor index of a graph. The following result can be easily obtained by derivation.

Lemma 2.1. *Let $f(x,y) := \frac{1}{\sqrt{x^2+y^2}}$ and $h(x,y) := f(x+1,y) - f(x,y)$, where $x, y \geq 1$. Then for a fixed y (or $x, resp.$), $f(x,y)$ is decreasing with respect to x (or y); for a fixed x, $h(x,y)$ is increasing with respect to y.*

Lemma 2.2. *Let $e = uv$ be an edge of a graph G such that $N_G(u) \cap N_G(v) = \emptyset$. Define G' as the graph obtained from G by removing the edge e and identifying v with u, and then attaching a leaf w to v (or u). If $d_G(u), d_G(v) \geq 2$, then ${}^{m}SO(G') < {}^{m}SO(G)$.*

Proof. Suppose $N_G(u)\backslash\{v\} = \{u_1, u_2, \ldots, u_x\}$ and $N_G(v)\backslash\{u\} = \{v_1, v_2, \ldots, v_y\}$, where $x, y \geq 1$. It follows from Lemma 2.1 that

$$
\begin{aligned}
& {}^{m}SO(G') - {}^{m}SO(G) \\
= \ & f(x+y+1,1) - f(x+1,y+1) + \sum_{i=1}^{x}[f(x+y+1, d_{G'}(u_i)) - f(x+1, d_G(u_i))] \\
& + \sum_{i=1}^{y}[f(x+y+1, d_{G'}(v_i)) - f(y+1, d_G(v_i))] \\
< \ & f(x+y+1,1) - f(x+1,y+1) \\
= \ & \frac{1}{\sqrt{x^2+y^2+2x+2y+2xy+2}} - \frac{1}{\sqrt{x^2+y^2+2x+2y+2}} \\
< \ & 0.
\end{aligned}
$$

□

The following lemma is a direct result of Lemma 2.2.

Lemma 2.3. *Let G be a graph with a leaf w and v be the neighbor of w with $d_G(v) \geq 3$. Let $u \in N_G(v) \setminus \{w\}$ and $G' = (G - uv) + uw$. Then ${}^{m}SO(G') > {}^{m}SO(G)$.*

Proof. By the definition of G', $N_{G'}(v) \cap N_{G'}(w) = \emptyset$, $d_{G'}(v) \geq 2$, and $d_{G'}(w) = 2$. Therefore, ${}^{m}SO(G') > {}^{m}SO(G)$ by Lemma 2.2. □

Lemma 2.4. *Let $P = vv_1 \cdots v_r$ be a pendant path of a graph G, where $r \geq 2$ and v is the origin of P with $d_G(v) = a \geq 3$. Suppose $u \in N_G(v) \setminus \{v_1\}$ and $d_G(u) = 2$. Let $G' = (G - uv) + uv_r$. Then ${}^{m}SO(G') > {}^{m}SO(G)$.*

Proof. By Lemma 2.1,

$$\begin{aligned}
& {}^{m}SO(G^{'}) - {}^{m}SO(G) \\
= & \sum_{x\in N_G(v)\setminus\{u,v_1\}} [f(d_G(x), d_G(v)-1) - f(d_G(x), d_G(v))] \\
& + f(d_G(u), 2) - f(d_G(u), a) + f(2,2) - f(1,2) + f(a-1,2) - f(a,2) \\
> & f(d_G(u), 2) - f(d_G(u), a) + f(2,2) - f(1,2) + f(a-1,2) - f(a,2) \\
= & f(a-1,2) - 2f(a,2) + \frac{2}{\sqrt{8}} - \frac{1}{\sqrt{5}}.
\end{aligned}$$

Let $g(a) = f(a-1,2) - 2f(a,2) = \frac{1}{\sqrt{(a-1)^2+4}} - \frac{2}{\sqrt{a^2+4}}$, where $a \geq 3$. We show that $g'(a) > 0$ for $a \in [3, +\infty)$. Since $g'(a) = \frac{2a}{(a^2+4)^{\frac{3}{2}}} - \frac{a-1}{((a-1)^2+4)^{\frac{3}{2}}}$, it suffices to show $\frac{(2a)^2}{(a^2+4)^3} > \frac{(a-1)^2}{((a-1)^2+4)^3}$, i.e., $(2a)^2((a-1)^2+4)^3 > (a^2+4)^3(a-1)^2$ for $a \geq 3$. Let $h(a) = (2a)^2((a-1)^2+4)^3 - (a^2+4)^3(a-1)^2$. By taking the derivatives, we get

$$h'(a) = 24a^7 - 154a^6 + 570a^5 - 1240a^4 + 1920a^3 - 1512a^2 + 776a + 128,$$

$$h''(a) = 168a^6 - 924a^5 + 2850a^4 - 4960a^3 + 5760a^2 - 3024a + 776,$$

$$h^{(3)}(a) = 1008a^5 - 4620a^4 + 11,400a^3 - 14,880a^2 + 11,520a - 3024,$$

$$h^{(4)}(a) = 5040a^4 - 18,480a^3 + 34,200a^2 - 29,760a + 11,520,$$

$$h^{(5)}(a) = 20,160a^3 - 55,440a^2 + 68,400a - 29,760,$$

$$h^{(6)}(a) = 60,480a^2 - 110,880a + 68,400.$$

Obviously, $h^{(6)}(a) > 0, \forall a \in R$. Combining it with $h^{(5)}(3) > 0$, we get $h^{(5)}(a) > 0$ for $a \geq 3$. Similarly, $h^{(4)}(3) > 0, h^{(3)}(3) > 0, h''(3) > 0, h'(3) > 0$, and $h(3) > 0$ yield that $h^{(4)}(a) > 0, h^{(3)}(a) > 0, h''(a) > 0, h'(a) > 0$, and $h(a) > 0$, i.e., $g'(a) > 0$ for $a \geq 3$. This implies $g(a)$ is strictly monotonically increasing in $[3, +\infty)$. Thus,

$$\begin{aligned}
& {}^{m}SO(G^{'}) - {}^{m}SO(G) \\
> & f(a-1,2) - 2f(a,2) + \frac{2}{\sqrt{8}} - \frac{1}{\sqrt{5}} \\
\geq & f(2,2) - 2f(3,2) + \frac{2}{\sqrt{8}} - \frac{1}{\sqrt{5}} \\
= & \frac{3}{\sqrt{8}} - \frac{2}{\sqrt{13}} - \frac{1}{\sqrt{5}} > 0.
\end{aligned}$$

□

3. Extremal values of the modified Sombor index in trees

With the graph transformations introduced in Section 2, we first investigate the extremal values of the modified Sombor index of trees with a fixed order. Let $\mathcal{T}_n$ denote the set of all trees of order n.

Theorem 3.1. *Let $T \in \mathcal{T}_n$, where $n \geq 4$. Then ${}^mSO(S_n) \leq {}^mSO(T) \leq {}^mSO(P_n)$, with equality iff $T \cong S_n$ or $T \cong P_n$.*

Proof. Let $T_0 \in \mathcal{T}_n$ be a tree with the maximum modified Sombor index. Let w be a leaf of T_0 and v be the neighbor of w. If $d_{T_0}(v) \geq 3$, by letting $u \in N_{T_0}(v) \setminus \{w\}$ and $T' = (T_0 - uv) + uw$, we get $T' \in \mathcal{T}_n$ and ${}^mSO(T') > {}^mSO(T_0)$ by Lemma 2.3, which is a contradiction. Thus, $d_{T_0}(v) = 2$. This implies that the length of every pendant path of T_0 (if it exists) is at least 2.

Suppose to the contrary that $T_0 \ncong P_n$. Then there must be two pendant paths P and P' with the same origin. Suppose $P = vv_1 \cdots v_r$ and $P' = vw_1 \cdots w_t$, where $d_{T_0}(v) \geq 3$. If follows from the above that $r, t \geq 2$. Let $T'' = (T_0 - vw_1) + v_r w_1$. Then $T'' \in \mathcal{T}_n$ and ${}^mSO(T'') > {}^mSO(T_0)$ by Lemma 2.4, which is a contradiction. Hence, $T_0 \cong P_n$.

Let $T_1 \in \mathcal{T}_n$ be a tree with the minimum modified Sombor index. If $T_1 \ncong S_n$, there must be an edge uv in T_1 with $d_{T_1}(u), d_{T_1}(v) \geq 2$. By Lemma 2.3, we can find a new tree $T' \in \mathcal{T}_n$ with ${}^mSO(T') < {}^mSO(T_1)$, which is a contradiction. Therefore, $T_1 \cong S_n$. □

Now we determine the trees in $\mathcal{T}_n$ with the second maximum and minimum modified Sombor indices. Let $S(a, b, c)$ be the tree such that $\Delta(S(a, b, c)) = 3$, v is the vertex of degree 3, and $S(a, b, c) - v = P_a \cup P_b \cup P_c$, where $1 \leq a \leq b \leq c$. Let $DS_{p,q}$ be the double star obtained from two stars S_{p+1} and S_{q+1} by adding an edge between the central vertices, where $p \geq q \geq 1$.

Theorem 3.2. *Suppose $T \in \mathcal{T}_n \setminus \{P_n\}$, where $n \geq 7$. Then ${}^mSO(T) \leq \frac{3}{\sqrt{5}} + \frac{3}{\sqrt{13}} + \frac{n-7}{\sqrt{8}}$, with equality if and only if $T \cong S(a, b, c)$, where $a \geq 2$.*

Proof. Let $T^* \in \mathcal{T}_n \setminus \{P_n\}$ be a tree with the maximum modified Sombor index. First, we show that $T^* \cong S(a, b, c)$, i.e., T^* has exactly three pendant paths.

Suppose T^* has at least four pendant paths. If there is a leaf w with the vertex v adjacent to it satisfying $d_{T^*}(v) \geq 3$, let $T' = (T^* - uv) + uw$, where $u \in N_{T^*}(v) \setminus \{w\}$. Then $T' \ncong P_n$ and ${}^mSO(T') > {}^mSO(T^*)$ by Lemma 2.3, which is a contradiction. Since w is an arbitrary leaf, this implies that the length of every pendant path is at least 2. In this case, let $P = vv_1 \cdots v_r$ and $P' = vw_1 \cdots w_t$ be two pendant paths with the same origin v and $T'' = (T^* - vw_1) + v_r w_1$. Then $T'' \ncong P_n$ and ${}^mSO(T'') > {}^mSO(T^*)$ by Lemma 2.4, which is a contradiction. Therefore, $T^* \cong S(a, b, c)$.

By direct calculation, ${}^mSO(S(1, 1, n-3)) = \frac{2}{\sqrt{10}} + \frac{1}{\sqrt{13}} + \frac{1}{\sqrt{5}} + \frac{n-5}{\sqrt{8}}$, ${}^mSO(S(1, b, n-b-2)) = \frac{1}{\sqrt{10}} + \frac{2}{\sqrt{13}} + \frac{2}{\sqrt{5}} + \frac{n-6}{\sqrt{8}}$ if $b \geq 2$, and ${}^mSO(S(a, b, c)) = \frac{3}{\sqrt{5}} + \frac{3}{\sqrt{13}} + \frac{n-7}{\sqrt{8}}$ if $a \geq 2$. Since $n \geq 7$, $\frac{2}{\sqrt{10}} + \frac{1}{\sqrt{13}} + \frac{1}{\sqrt{5}} + \frac{n-5}{\sqrt{8}} < \frac{1}{\sqrt{10}} + \frac{2}{\sqrt{13}} + \frac{2}{\sqrt{5}} + \frac{n-6}{\sqrt{8}} < \frac{3}{\sqrt{5}} + \frac{3}{\sqrt{13}} + \frac{n-7}{\sqrt{8}}$. Therefore, $T^* \cong S(a, b, c)$, where $a \geq 2$. □

Theorem 3.3. *Let $T \in \mathcal{T}_n \setminus \{S_n\}$, where $n \geq 4$. Then ${}^mSO(T) \geq \frac{n-3}{\sqrt{n^2-4n+5}} + \frac{1}{\sqrt{5}} + \frac{1}{\sqrt{n^2-4n+8}}$, with equality if and only if $T \cong DS_{n-3,1}$.*

Proof. Let d be the diameter of T. Then $d \geq 3$ since $T \ncong S_n$. We consider the following two cases.

Case 1. $d = 3$.

In the case where $T \cong DS_{p,q}$, since $p \geq q$ and $n = p + q + 2$, we have $q \leq \frac{n}{2} - 1$.

First we consider the function $g(q) = \frac{n-q-2}{\sqrt{(n-q-1)^2+1}} + \frac{q}{\sqrt{(q+1)^2+1}}$, where $1 \leq q \leq \frac{n}{2} - 1$. By calculation, $g'(q) = \frac{q+2}{((q+2-1)^2+1)^{\frac{3}{2}}} - \frac{n-q}{((n-q-1)^2+1)^{\frac{3}{2}}}$. Notice that $q + 2 \leq n - q$. We define $h(t) = \frac{t}{((t-1)^2+1)^{\frac{3}{2}}}$. Then

$h'(t) = \frac{-2t^2+t+2}{[(t-1)^2+1]^{\frac{5}{2}}}$. Obviously, $h'(t) < 0$ if $t > \frac{1+\sqrt{17}}{4}$. This indicates that $h(t)$ is strictly monotonically decreasing in $[\frac{1+\sqrt{17}}{4}, +\infty)$. When $1 \le q \le \frac{n}{2} - 1$, $3 \le q + 2 \le n - q$. Therefore, $h(q + 2) \ge h(n - q)$, with equality if and only if $q + 2 = n - q$, i.e., $q = \frac{n}{2} - 1$. This implies $g'(q) \ge 0$ if $1 \le q \le \frac{n}{2} - 1$, and $g'(q) = 0$ if and only if $q = \frac{n}{2} - 1$. Thus, $g(q) \ge g(1)$ if $1 \le q \le \frac{n}{2} - 1$, with equality if and only if $q = 1$.

Now we consider the function $r(q) = \frac{1}{\sqrt{(n-q-1)^2+(q+1)^2}}$, where $1 \le q \le \frac{n}{2} - 1$. It is easy to verify that $r(q)$ is strictly monotonically increasing in $[1, \frac{n}{2} - 1]$. Therefore, $r(q) \ge r(1)$, with equality if and only if $q = 1$.

Based on the above,

$$\begin{aligned} {}^{m}SO(T) &= \frac{p}{\sqrt{(p+1)^2+1}} + \frac{q}{\sqrt{(q+1)^2+1}} + \frac{1}{\sqrt{(n-q-1)^2+(q+1)^2}} \\ &= g(q) + r(q) \\ &\ge g(1) + r(1) \\ &= \frac{n-3}{\sqrt{n^2-4n+5}} + \frac{1}{\sqrt{5}} + \frac{1}{\sqrt{n^2-4n+8}}, \end{aligned}$$

with equality if and only if $q = 1$, i.e., $T \cong DS_{n-3,1}$.

Case 2. $d \ge 4$.

Since T is a tree, by recursively using graph transformations in Lemma 2.2, we can get a new tree T' of diameter 3 such that ${}^{m}SO(T') < {}^{m}SO(T)$. By Case 1, ${}^{m}SO(T') \ge {}^{m}SO(DS_{n-3,1})$. This yields ${}^{m}SO(T) > {}^{m}SO(DS_{n-3,1})$. □

Let $\mathcal{TP}_p$ be the set of all trees with p number of pendant vertices. The following theorem determines the unique tree attaining the minimum modified Sombor index among $\mathcal{TP}_p$.

Theorem 3.4. *Let $T \in \mathcal{TP}_p$, where $p \ge 2$. Then ${}^{m}SO(T) \ge \frac{p}{\sqrt{p^2+1}}$, with equality if and only if $T \cong S_{p+1}$.*

Proof. Let $T_0 \in \mathcal{TP}_p$ be a tree with the minimum modified Sombor index. First, we show that there is no vertex of degree 2 in T_0.

Suppose to the contrary that there is a vertex of degree 2 in T_0, say v, and $N_{T_0}(v) = \{v_1, v_2\}$. Here we suppose $d_{T_0}(v_1) \ge d_{T_0}(v_2)$ without loss of generality. Let $T_1 = (T_0 - v) + v_1v_2$. Then $T_1 \in \mathcal{TP}_p$ and ${}^{m}SO(T_0) - {}^{m}SO(T_1) = f(d_{T_0}(v_1), 2) + f(d_{T_0}(v_2), 2) - f(d_{T_0}(v_1), d_{T_0}(v_2))$. By Lemma 2.1, if $d_{T_0}(v_2) \ge 2$, then ${}^{m}SO(T_0) - {}^{m}SO(T_1) \ge f(d_{T_0}(v_2), 2) > 0$; if $d_{T_0}(v_2) = 1$ and $d_{T_0}(v_1) \ge 2$, then ${}^{m}SO(T_0) - {}^{m}SO(T_1) \ge f(d_{T_0}(v_1), 2) > 0$; if $d_{T_0}(v_1) = d_{T_0}(v_2) = 1$, then ${}^{m}SO(T_0) - {}^{m}SO(T_1) = \frac{2}{\sqrt{5}} - \frac{1}{\sqrt{2}} > 0$. This contradicts the choice of T_0, which implies that T_0 has no vertex of degree 2.

To show $T_0 \cong S_{p+1}$, it suffices to show there is only one non-pendant vertex in T_0. Suppose T_0 has at least two non-pendant vertices. Then there are two vertices u and w satisfying $d_{T_0}(u), d_{T_0}(w) \ge 3$ and $uw \in E(T_0)$. Let $N_{T_0}(u) \setminus \{w\} = \{u_1, u_2, \ldots, u_x\}$ and $N_{T_0}(w) \setminus \{u\} = \{w_1, w_2, \ldots, w_y\}$, where $x, y \ge 2$. Define $T_2 = (T_0 - w) + \{uw_1, \ldots, uw_y\}$. Then $T_2 \in \mathcal{TP}_p$ and

$$\begin{aligned} &{}^{m}SO(T_0) - {}^{m}SO(T_2) \\ = \; & f(x+1, y+1) + \sum_{i=1}^{x}[f(x+1, d_{T_0}(u_i)) - f(x+y, d_{T_0}(u_i))] \end{aligned}$$

$$+\sum_{i=1}^{y}[f(y+1,d_{T_0}(w_i))-f(x+y,d_{T_0}(w_i))]$$
$$> f(x+1,y+1)$$
$$> 0,$$

which is a contradiction to the choice of T_0. Therefore, $T_0 \cong S_{p+1}$. □

4. Extremal values of the modified Sombor index in molecular trees

In this section, we determine the extremal values of the modified Sombor index of molecular trees with a fixed order. Denote by $\mathcal{MT}_n$ the set of all molecular trees of order n. Since $P_n \in \mathcal{MT}_n$, by Theorem 3.1, we easily have the following result.

Theorem 4.1. *P_n is the unique graph with the maximum modified Sombor index among $\mathcal{MT}_n$.*

To determine the tree in $\mathcal{MT}_n$ with the minimum modified Sombor index, we give the following lemma. The proof of it refers to that in [3] to some extent and we investigate it in greater detail.

Lemma 4.1. *Suppose T is a tree having the minimum modified Sombor index among $\mathcal{MT}_n$. For $1 \leq i \leq 4$, let V_i be the set of all vertices in T with degree i and $|V_i|$ be the cardinality of V_i. Then we have:*

(1) For arbitrary two vertices u and v with $u \in V_2$ and $v \in V_2 \cup V_3$, $uv \notin E(T)$;

(2) $|V_2| \leq 1$;

(3) $|V_3| \leq 1$;

(4) $|V_2| \cdot |V_3| = 0$.

Proof. (1) can be easily obtained by Lemma 2.2.

(2) Suppose to the contrary that $|V_2| \geq 2$. Let $u, v \in V_2$ and $u \neq v$. By (1), $uv \notin E(T)$. Let $P = uu_1 \cdots v_1v$ be the path connecting u and v in T, $N_T(u) \setminus \{u_1\} = \{u_2\}$, and $N_T(v) \setminus \{v_1\} = \{v_2\}$. Since $u, v \in V_2$, by (1), $u_1, v_1 \notin V_2 \cup V_3$. Therefore, $u_1, v_1 \in V_4$. Let $T' = (T - uu_2) + vu_2$. Then $T' \in \mathcal{MT}_n$. By Lemma 2.1,

$$\begin{aligned}
{}^{m}SO(T') - {}^{m}SO(T) &= f(3,4) - f(2,4) + f(3,d_T(v_2)) - f(2,d_T(v_2)) \\
&\quad + f(3,d_T(u_2)) - f(2,d_T(u_2)) + f(1,4) - f(2,4) \\
&= h(2,4) + h(2,d_T(v_2)) + h(2,d_T(u_2)) - h(1,4) \\
&\leq 3h(2,4) - h(1,4) \\
&< 0,
\end{aligned}$$

which is contrary to the definition of T.

(3) Suppose to the contrary that $|V_3| \geq 2$. Let $u, v \in V_3$ and $u \neq v$. Suppose $uv \notin E(T)$. Let $P = uu_1 \cdots v_1v$ be the path connecting u and v in T, $N_T(u) \setminus \{u_1\} = \{u_2, u_3\}$, and $N_T(v) \setminus \{v_1\} = \{v_2, v_3\}$. Since $u, v \in V_3$, by (1), $u_i, v_i \notin V_2$ for $i = 1, 2, 3$. Therefore, $u_1, v_1 \in V_3 \cup V_4$. Suppose $\{u_2, u_3, v_2, v_3\} \not\subseteq V_1$. Without loss of generality, we suppose $u_2 \notin V_1$. Then $u_2 \in V_3 \cup V_4$. Let $T' = (T - uu_3) + vu_3$. Then $T' \in \mathcal{MT}_n$ and by Lemma 2.1,

$${}^{m}SO(T') - {}^{m}SO(T)$$

$$
\begin{aligned}
&= f(4,d_T(u_3)) - f(3,d_T(u_3)) + \sum_{i=1}^{3}[f(4,d_T(v_i)) - f(3,d_T(v_i))] \\
&\quad + \sum_{i=1}^{2}[f(2,d_T(u_i)) - f(3,d_T(u_i))] \\
&= h(3,d_T(u_3)) + \sum_{i=1}^{3} h(3,d_T(v_i)) - \sum_{i=1}^{2} h(2,d_T(u_i)) \\
&\le h(3,4) + 3h(3,4) - 2h(2,3) \\
&< 0,
\end{aligned}
$$

which is a contradiction.

Suppose $\{u_2, u_3, v_2, v_3\} \subseteq V_1$. Let $T' = (T - uu_3) + vu_3$. Then $T' \in \mathcal{MT}_n$ and by Lemma 2.1,

$$
\begin{aligned}
&{}^{m}SO(T') - {}^{m}SO(T) \\
&= f(4,d_T(v_1)) - f(3,d_T(v_1)) + f(2,d_T(u_1)) - f(3,d_T(u_1)) \\
&\quad + 3(f(4,1) - f(3,1)) + f(2,1) - f(3,1) \\
&= h(3,d_T(v_1)) - h(2,d_T(u_1)) + 3h(3,1) - h(2,1) \\
&\le h(3,4) - h(2,3) + 3h(3,1) - h(2,1) \\
&< 0,
\end{aligned}
$$

which is a contradiction.

Now we consider the case $uv \in E(T)$. Let $N_T(u) \setminus \{v\} = \{u_1, u_2\}$ and $N_T(v) \setminus \{u\} = \{v_1, v_2\}$. By (1), $u_i, v_i \notin V_2$ for $i = 1, 2$. Suppose $\{u_1, u_2, v_1, v_2\} \nsubseteq V_1$. Without loss of generality, we suppose $u_2 \notin V_1$. Then $u_2 \in V_3 \cup V_4$. Let $T' = (T - uu_1) + vu_1$. Then $T' \in \mathcal{MT}_n$ and by Lemma 2.1,

$$
\begin{aligned}
&{}^{m}SO(T') - {}^{m}SO(T) \\
&= f(4,2) - f(3,3) + \sum_{i=1}^{2}[f(4,d_T(v_i)) - f(3,d_T(v_i))] \\
&\quad + f(4,d_T(u_1)) - f(3,d_T(u_1)) + f(2,d_T(u_2)) - f(3,d_T(u_2)) \\
&= f(4,2) - f(3,3) + \sum_{i=1}^{2} h(3,d_T(v_i)) + h(3,d_T(u_1)) - h(2,d_T(u_2)) \\
&\le f(4,2) - f(3,3) + 3h(3,4) - h(2,3) \\
&< 0,
\end{aligned}
$$

which is a contradiction.

Now suppose $\{u_1, u_2, v_1, v_2\} \subseteq V_1$. Let $T' = (T - uu_1) + vu_1$. Then $T' \in \mathcal{MT}_n$ and ${}^{m}SO(T') - {}^{m}SO(T) = f(4,2) - f(3,3) + 3[f(4,1) - f(3,1)] + f(2,1) - f(3,1) < 0$, which is a contradiction.

(4) Suppose to the contrary that $|V_2| \cdot |V_3| \neq 0$. Then $|V_2| = |V_3| = 1$ by (2) and (3). Let $V_2 = \{u\}$ and $V_3 = \{v\}$. By (1), $uv \notin E(T)$. Let $P = uu_1 \cdots v_1 v$ be the path connecting u and v in T, $N_T(u) \setminus \{u_1\} = \{u_2\}$, and $N_T(v) \setminus \{v_1\} = \{v_2, v_3\}$. By (1), $u_1 \notin V_2 \cup V_3$. Thus, $u_1 \in V_4$. Let $T' = (T - uu_2) + vu_2$. Then $T' \in \mathcal{MT}_n$ and by Lemma 2.1,

$$
{}^{m}SO(T') - {}^{m}SO(T)
$$

$$
\begin{aligned}
&= f(4,d_T(u_2)) - f(2,d_T(u_2)) + \sum_{i=1}^{3}[f(4,d_T(v_i)) - f(3,d_T(v_i))] \\
&\quad + f(1,4) - f(2,4) \\
&= h(3,d_T(u_2)) + h(2,d_T(u_2)) + \sum_{i=1}^{3} h(3,d_T(v_i)) - h(1,4) \\
&\leq h(3,4) + h(2,4) + 3h(3,4) - h(1,4) \\
&< 0,
\end{aligned}
$$

which is the final contradiction. □

For a tree $T \in \mathcal{MT}_n$ and $1 \leq i \leq 4$, let V_i be the set of all vertices in T with degree i. Let $\mathcal{MT}_n^*$ be the set of all molecular trees T of order n such that $|V_2| + |V_3| \leq 1$ and for every pendant vertex, the vertex adjacent to it is in V_4 in T. Let T_1 be the molecular tree of order 10 such that $|V_1| = 7$, $|V_2| = 0$, $|V_3| = 1$, $|V_4| = 2$, and the unique vertex of degree 3 is adjacent to exactly one pendant vertex.

Theorem 4.2. *Suppose T is a tree in $\mathcal{MT}_n$ with the minimum modified Sombor index, where $n \geq 5$. For $n = 6$, $T \cong DS_{3,1}$. For $n = 7$, $T \cong DS_{3,2}$. For $n = 10$, $T \cong T_1$. For $n \neq 6,7,10$, $T \in \mathcal{MT}_n^*$ and*

$$
{}^{m}SO(T) = \begin{cases} \frac{2k+2}{\sqrt{17}} + \frac{k-1}{\sqrt{32}}, & n = 3k+2\ (k \geq 1), \\ \frac{2k+1}{\sqrt{17}} + \frac{k-4}{\sqrt{32}} + \frac{3}{5}, & n = 3k+1\ (k \geq 4), \\ \frac{2k}{\sqrt{17}} + \frac{k-3}{\sqrt{32}} + \frac{2}{\sqrt{20}}, & n = 3k\ (k \geq 3). \end{cases}
$$

Proof. Let $|V_i|$ be the cardinality of V_i. Then $|V_1|+|V_2|+|V_3|+|V_4| = n$ and $|V_1|+2|V_2|+3|V_3|+4|V_4| = 2(n-1)$. Thus, $|V_2| + 2|V_3| + 3|V_4| = n - 2$. By Lemma 4.1, $|V_2| + |V_3| \leq 1$.

If $n = 3k + 2$, where $k \geq 1$, then $|V_2| + 2|V_3| + 3|V_4| = 3k$. Since $|V_2| + |V_3| \leq 1$, it follows that $|V_2| = |V_3| = 0$. Therefore, $T \in \mathcal{MT}_n^*$, $|V_1| = 2k + 2$, $|V_4| = k$, and ${}^{m}SO(T) = |V_1|f(1,4) + (n-1-|V_1|)f(4,4) = \frac{2k+2}{\sqrt{17}} + \frac{k-1}{\sqrt{32}}$.

If $n = 3k + 1$, where $k \geq 2$, then $|V_2| + 2|V_3| + 3|V_4| = 3k - 1$. Since $|V_2| + |V_3| \leq 1$, it follows that $|V_2| = 0$ and $|V_3| = 1$. Therefore, $|V_1| = 2k + 1$, $|V_4| = k - 1$. Let $V_3 = \{u\}$. If $k = 2$, it is obvious that $T \cong DS_{3,2}$.

Now suppose $k \geq 3$. If u is adjacent to exactly one pendant vertex, then each of the rest of the pendant vertices is adjacent to a vertex in V_4. Thus, ${}^{m}SO(T) = f(1,3) + (|V_1| - 1)f(1,4) + 2f(3,4) + (n-3-|V_1|)f(4,4) = \frac{1}{\sqrt{10}} + \frac{2k}{\sqrt{17}} + \frac{2}{5} + \frac{k-3}{\sqrt{32}}$.

If u is adjacent to two pendant vertices, then ${}^{m}SO(T) = 2f(1,3) + (|V_1| - 2)f(1,4) + f(3,4) + (n-2-|V_1|)f(4,4) = \frac{2}{\sqrt{10}} + \frac{2k-1}{\sqrt{17}} + \frac{1}{5} + \frac{k-2}{\sqrt{32}}$.

If there is no pendant vertex adjacent to u, then ${}^{m}SO(T) = |V_1|f(1,4) + 3f(3,4) + (n-4-|V_1|)f(4,4) = \frac{2k+1}{\sqrt{17}} + \frac{3}{5} + \frac{k-4}{\sqrt{32}}$.

Since $k \geq 3$, we get $\frac{2k+1}{\sqrt{17}} + \frac{3}{5} + \frac{k-4}{\sqrt{32}} < \frac{1}{\sqrt{10}} + \frac{2k}{\sqrt{17}} + \frac{2}{5} + \frac{k-3}{\sqrt{32}} < \frac{2}{\sqrt{10}} + \frac{2k-1}{\sqrt{17}} + \frac{1}{5} + \frac{k-2}{\sqrt{32}}$. Notice that T has the minimum modified Sombor index among $\mathcal{MT}_n$ and there are only two vertices in V_4 if $k = 3$. Therefore, u is adjacent to exactly one pendant vertex if $k = 3$, i.e., $T \cong T_1$ if $n = 10$; if $k \geq 4$, no pendant vertex is adjacent to u, i.e., $T \in \mathcal{MT}_n^*$ and ${}^{m}SO(T) = \frac{2k+1}{\sqrt{17}} + \frac{3}{5} + \frac{k-4}{\sqrt{32}}$.

If $n = 3k$, where $k \geq 2$, then $|V_2|+2|V_3|+3|V_4| = 3k-2$. Since $|V_2|+|V_3| \leq 1$, it follows that $|V_2| = 1$ and $|V_3| = 0$. Therefore, $|V_1| = 2k$, $|V_4| = k - 1$. Let $V_2 = \{u\}$. If $k = 2$, it is obvious that $T \cong DS_{3,1}$.

Now suppose $k \geq 3$. If u is adjacent to exactly one pendant vertex, then ${}^{m}SO(T) = f(1,2) + (|V_1| - 1)f(1,4) + f(2,4) + (n-2-|V_1|)f(4,4) = \frac{1}{\sqrt{5}} + \frac{2k-1}{\sqrt{17}} + \frac{1}{\sqrt{20}} + \frac{k-2}{\sqrt{32}}$. If no pendant vertex is adjacent to u, then ${}^{m}SO(T) = |V_1|f(1,4) + 2f(2,4) + (n-3-|V_1|)f(4,4) = \frac{2k}{\sqrt{17}} + \frac{2}{\sqrt{20}} + \frac{k-3}{\sqrt{32}}$. Since $k \geq 3$, we get $\frac{2k}{\sqrt{17}} + \frac{2}{\sqrt{20}} + \frac{k-3}{\sqrt{32}} < \frac{1}{\sqrt{5}} + \frac{2k-1}{\sqrt{17}} + \frac{1}{\sqrt{20}} + \frac{k-2}{\sqrt{32}}$. Notice that T has the minimum modified Sombor index. Thus, there is no pendant vertex adjacent to u, i.e., $T \in \mathcal{MT}_n^*$ and ${}^{m}SO(T) = \frac{2k}{\sqrt{17}} + \frac{2}{\sqrt{20}} + \frac{k-3}{\sqrt{32}}$. □

Remark 4.1. In Theorem 4.2, we characterize the unique graph with the minimum modified Sombor index among all chemical graphs of order n and size $m = n-1$, where $n \geq 5$. By taking $\beta_{i,j} = \frac{1}{\sqrt{i^2+j^2}}$ in Theorem 1 in [24], Albalahi et al. actually gave a more general result about the minimum modified Sombor index of chemical graphs of order n and size m, where $n-1 \leq m \leq 2n$ and $n \geq 13$.

5. Conclusions

In chemical graph theory, one of the most common problems is to determine the extremal values of various topological indices because of their applications in Quantitative structure-activity (structure-property) relationships (QSAR/QSPR). As a recently introduced concept, the Sombor index has been extensively studied both in chemistry and mathematics. Kulli and Gutman [9] proposed its modified version. In this paper, we consider the extremal values of the modified Sombor index for trees. Some graph transformations are introduced to compare the modified Sombor indices of two graphs. With these transformations, we determine the first two maximum and minimum values of all trees of order n. We also find that S_{p+1} is the unique tree that minimizes ${}^{m}SO$ among all trees with p pendant vertices. The molecular trees with the maximum and minimum modified Sombor indices are also considered. It is interesting to consider the extremal values of the modified Sombor index in the set of other classic graphs, such as cacti, quasi-trees, molecular trees with given graph parameters, and k-cyclic (molecular) graphs. We will investigate this in the future.

Author contributions

Kun Wang: Investigation, Writing–original draft; Wenjie Ning: Conceptualization, Project administration, Supervision; Yuheng Song: Validation, Writing–review and editing.

Use of Generative-AI tools declaration

The authors declare they have not used Artiffcial Intelligence (AI) tools in the creation of this article.

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Conflict of interest

All authors declare no conflicts of interest in this paper.

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