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Extremal (Molecular) Trees with Respect to Multiplicative Sombor Indices

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Abstract Topological indices are a class of numerical invariants that can be used to predict the physicochemical properties of compounds and are widely used in quantum chemistry, molecular biology and other research field. For a (molecular) graph G with vertex set $V(G)$ and edge set $E(G)$, the Sombor index is defined as $\mathrm{SO}(G) = \sum_{uv\in E(G)} \sqrt{d_G^2(u) + d_G^2(v)}$, where $d_G(u)$ denotes the degree of vertex u in G. Accordingly, the multiplicative Sombor index is defined as $\prod_{\mathrm{SO}}(G) = \prod_{uv\in E(G)} \sqrt{d_G^2(u) + d_G^2(v)}$. A molecular tree is a tree with maximum degree $\Delta \le 4$. In this paper, we first determine the maximum molecular trees with respect to multiplicative Sombor index. Then we determine the first thirteen minimum (molecular) trees with respect to multiplicative Sombor index.

Keywords tree; molecular tree; multiplicative Sombor index; extremal value

MR(2020) Subject Classification 05C05; 05C09; 05C92

1. Introduction

In this paper, we only consider simple connected graphs. Let $N_G(u)$ be the set of vertices that are neighbors of the vertex u. Then $|N_G(u)|$ is the degree of vertex u, denoted by $d_G(u)$ or $d(u)$. We call a vertex u in graph G a pendent vertex (branching vertex) if $d_G(u) = 1$ ($d_G(u) \ge 3$). Denote by n_i the number of vertices with degree i, $m_{i,j}$ the number of edges with degree of end-ponits i and j. A molecular tree is a tree with maximum degree $\Delta \le 4$. For all notations and terminology used, but not defined here, we refer to [1]. We will omit the subscript G or T if the graph is clear from the context.

In 2020, Gutman proposed a new graphical invariant: Sombor index (SO) [2], which is defined as

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

The Sombor index differs from other vertex-degree-based indices because it has a peculiar geometric interpretation. After the Sombor index was conceived in [2], the evident task was to

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determine its main mathematical properties and chemical applications, see [3–8] and the references within. A nearly complete survey of these researches is found in [9].

Accordingly, the multiplicative Sombor index ($\prod_{\rm SO}$) is defined as

$$\prod\nolimits_{\rm SO}(G)=\prod_{uv\in E(G)}\sqrt{d_G^2(u)+d_G^2(v)}.$$

For the multiplicative Sombor index, Liu [10] had conceived the extremal values of graphs. Recently, Deng et al. [11] treated the maximum Sombor index of molecular trees. Liu et al. [12] ordered the minimum molecular trees with respect to Sombor index. As an extension of results of [11, 12], we consider the multiplicative Sombor index. In this paper, we first determine the maximum molecular trees with respect to multiplicative Sombor index. Then we determine the first thirteen minimum (molecular) trees with respect to multiplicative Sombor index.

2. Maximum molecular trees

Denote by $\mathcal{CT}_n$ the set of molecular trees with n vertices, $\mathcal{CT}_n^*$ the set of molecular trees with n vertices and $n_2+n_3\le 1$.

Lemma 2.1 *Let $T\in\mathcal{CT}_n$ and $n_3(T)\ge 2$. Then T is not a maximum molecular tree with respect to multiplicative Sombor index in $\mathcal{CT}_n$.*

Proof Suppose that $d(u)=d(v)=3$, $N_T(u)=\{u_1,u_2,u_3\}$, $N_T(v)=\{v_1,v_2,v_3\}$. Since T is a tree, there exists a unique path between u and v. We suppose the unique path from u to v goes through u_2 and v_2. Without loss of generality, we suppose $d(u_1)\le d(u_3)$. Let $T^*=T-\{uu_1\}+\{vu_1\}$. Then $T^*\in\mathcal{CT}_n$.

Case 1. $u\nsim v$.

$$\begin{aligned}\frac{\prod_{\rm SO}(T^*)}{\prod_{\rm SO}(T)}&=\frac{\sqrt{16+d^2(u_1)}\sqrt{4+d^2(u_2)}\sqrt{4+d^2(u_3)}\prod_{i=1}^3\sqrt{16+d^2(v_i)}}{\prod_{i=1}^3\sqrt{9+d^2(u_i)}\prod_{i=1}^3\sqrt{9+d^2(v_i)}}\\&=\frac{\sqrt{1+\frac{7}{9+d^2(u_1)}}\prod_{i=1}^3\sqrt{1+\frac{7}{9+d^2(v_i)}}}{\sqrt{1+\frac{5}{4+d^2(u_2)}}\sqrt{1+\frac{5}{4+d^2(u_3)}}}.\end{aligned}$$

Since $d(u_1)\le d(u_3)$ and $d(u_2)\ge 2$,

(1) If $d(u_2)\ge 2$ and $d(u_3)=1$, then $d(u_1)=1$ and $d(v_i)\le 4$ $(i=1,2,3)$. Then

$$\frac{\prod_{\rm SO}(T^*)}{\prod_{\rm SO}(T)}\ge\frac{\sqrt{1+\frac{7}{9+1^2}}\prod_{i=1}^3\sqrt{1+\frac{7}{9+4^2}}}{\sqrt{1+\frac{5}{4+2^2}}\sqrt{1+\frac{5}{4+1^2}}}>1.$$

(2) If $d(u_2)\ge 2$ and $d(u_3)=2$, then $d(u_1)\le 2$ and $d(v_i)\le 4$ $(i=1,2,3)$. Then

$$\frac{\prod_{\rm SO}(T^*)}{\prod_{\rm SO}(T)}\ge\frac{\sqrt{1+\frac{7}{9+2^2}}\prod_{i=1}^3\sqrt{1+\frac{7}{9+4^2}}}{\sqrt{1+\frac{5}{4+2^2}}\sqrt{1+\frac{5}{4+2^2}}}>1.$$

(3) If $d(u_2) \geq 2$ and $d(u_3) = 3$, then $d(u_1) \leq 3$ and $d(v_i) \leq 4$ $(i = 1, 2, 3)$. Then

$$\frac{\prod_{\mathrm{SO}}(T^*)}{\prod_{\mathrm{SO}}(T)} \geq \frac{\sqrt{1+\frac{7}{9+3^2}}\prod_{i=1}^{3}\sqrt{1+\frac{7}{9+4^2}}}{\sqrt{1+\frac{5}{4+2^2}}\sqrt{1+\frac{5}{4+3^2}}} > 1.$$

(4) If $d(u_2) \geq 2$ and $d(u_3) = 4$, then $d(u_1) \leq 4$ and $d(v_i) \leq 4$ $(i = 1, 2, 3)$. Then

$$\frac{\prod_{\mathrm{SO}}(T^*)}{\prod_{\mathrm{SO}}(T)} \geq \frac{\sqrt{1+\frac{7}{9+4^2}}\prod_{i=1}^{3}\sqrt{1+\frac{7}{9+4^2}}}{\sqrt{1+\frac{5}{4+2^2}}\sqrt{1+\frac{5}{4+4^2}}} > 1.$$

Case 2. $u \sim v$.

$$\begin{aligned}\frac{\prod_{\mathrm{SO}}(T^*)}{\prod_{\mathrm{SO}}(T)} &= \frac{\sqrt{4+16}\sqrt{16+d^2(u_1)}\sqrt{4+d^2(u_3)}\sqrt{16+d^2(v_1)}\sqrt{16+d^2(v_3)}}{\sqrt{9+9}\sqrt{9+d^2(u_1)}\sqrt{9+d^2(u_3)}\sqrt{9+d^2(v_1)}\sqrt{9+d^2(v_3)}} \\ &= \frac{\sqrt{\frac{10}{9}}\sqrt{1+\frac{7}{9+d^2(u_1)}}\sqrt{1+\frac{7}{9+d^2(v_1)}}\sqrt{1+\frac{7}{9+d^2(v_3)}}}{\sqrt{1+\frac{5}{4+d^2(u_3)}}}.\end{aligned}$$

Since $d(u_1) \leq 4$, $d(v_1) \leq 4$, $d(v_3) \leq 4$ and $d(u_3) \geq 1$. Let $d(u_1) = d(v_1) = d(v_3) = 4$ and $d(u_3) = 1$. We can desire the minimum value of $\frac{\prod_{\mathrm{SO}}(T^*)}{\prod_{\mathrm{SO}}(T)}$, thus

$$\frac{\prod_{\mathrm{SO}}(T^*)}{\prod_{\mathrm{SO}}(T)} \geq \frac{\sqrt{\frac{10}{9}}\sqrt{1+\frac{7}{9+4^2}}\sqrt{1+\frac{7}{9+4^2}}\sqrt{1+\frac{7}{9+4^2}}}{\sqrt{1+\frac{5}{4+1^2}}} > 1.$$

As required, we complete the proof. □

Lemma 2.2 *Let $T \in \mathcal{CT}_n$ and $n_2(T) \geq 2$. Then T is not a maximum molecular tree with respect to multiplicative Sombor index in $\mathcal{CT}_n$.*

Proof Suppose that $d(u) = d(v) = 2$, $N_T(u) = \{u_1, u_2\}$, $N_T(v) = \{v_1, v_2\}$. We suppose the unique path from u to v goes through u_2 and v_2. Note that $u_2 \geq 2$. Let $T^* = T - \{uu_1\} + \{vu_1\}$. Then $T^* \in \mathcal{CT}_n$.

Case 1. $u \nsim v$.

$$\begin{aligned}\frac{\prod_{\mathrm{SO}}(T^*)}{\prod_{\mathrm{SO}}(T)} &= \frac{\sqrt{9+d^2(u_1)}\sqrt{1+d^2(u_2)}\sqrt{9+d^2(v_1)}\sqrt{9+d^2(v_2)}}{\sqrt{4+d^2(u_1)}\sqrt{4+d^2(u_2)}\sqrt{4+d^2(v_1)}\sqrt{4+d^2(v_2)}} \\ &= \frac{\sqrt{1+\frac{5}{4+d^2(u_1)}}\sqrt{1+\frac{5}{4+d^2(v_1)}}\sqrt{1+\frac{5}{4+d^2(v_2)}}}{\sqrt{1+\frac{3}{1+d^2(u_2)}}}.\end{aligned}$$

Since $d(u_2) \geq 2$, $d(u_1) \leq 4$, $d(v_1) \leq 4$, $d(v_2) \leq 4$. Let $d(u_1) = d(v_1) = d(v_2) = 4$ and $d(u_2) = 2$. We can desire the minimum value of $\frac{\prod_{\mathrm{SO}}(T^*)}{\prod_{\mathrm{SO}}(T)}$, thus

$$\frac{\prod_{\mathrm{SO}}(T^*)}{\prod_{\mathrm{SO}}(T)} \geq \frac{\sqrt{1+\frac{5}{4+4^2}}\sqrt{1+\frac{5}{4+4^2}}\sqrt{1+\frac{5}{4+4^2}}}{\sqrt{1+\frac{3}{1+2^2}}} > 1.$$

Case 2. $u \sim v$.

$$\frac{\prod_{\mathrm{SO}}(T^*)}{\prod_{\mathrm{SO}}(T)} = \frac{\sqrt{1+9}\sqrt{9+d^2(u_1)}\sqrt{9+d^2(v_1)}}{\sqrt{4+4}\sqrt{4+d^2(u_1)}\sqrt{4+d^2(v_1)}} > 1.$$

As required, we complete the proof. □

Lemma 2.3 *Let $T \in \mathcal{CT}_n$ and $n_2(T) \geq 1$, $n_3(T) \geq 1$. Then T is not a maximum molecular tree with respect to multiplicative Sombor index in $\mathcal{CT}_n$.*

Proof Suppose that $d(u) = 2$, $d(v) = 3$, $N_T(u) = \{u_1, u_2\}$, $N_T(v) = \{v_1, v_2, v_3\}$. We suppose that the unique path from u to v goes through u_2 and v_2. Note that $u_2 \geq 2$. Let $T^* = T - \{uu_1\} + \{vu_1\}$. Then $T^* \in \mathcal{CT}_n$.

Case 1. $u \nsim v$.

$$\begin{aligned}\frac{\prod_{\mathrm{SO}}(T^*)}{\prod_{\mathrm{SO}}(T)} &= \frac{\sqrt{16+d^2(u_1)}\sqrt{1+d^2(u_2)}\prod_{i=1}^{3}\sqrt{16+d^2(v_i)}}{\prod_{i=1}^{2}\sqrt{4+d^2(u_i)}\prod_{i=1}^{3}\sqrt{9+d^2(v_i)}}\\ &= \frac{\sqrt{1+\frac{12}{4+d^2(u_1)}}\prod_{i=1}^{3}\sqrt{1+\frac{7}{9+d^2(v_i)}}}{\sqrt{1+\frac{3}{1+d^2(u_2)}}}.\end{aligned}$$

Since $d(u_2) \geq 2$, $d(u_1) \leq 4$, $d(v_i) \leq 4$ $(i = 1, 2, 3)$. Let $d(u_1) = d(v_1) = d(v_2) = d(v_3) = 4$ and $d(u_2) = 2$. We can desire the minimum value of $\frac{\prod_{\mathrm{SO}}(T^*)}{\prod_{\mathrm{SO}}(T)}$, thus

$$\frac{\prod_{\mathrm{SO}}(T^*)}{\prod_{\mathrm{SO}}(T)} \geq \frac{\sqrt{1+\frac{12}{4+4^2}}\prod_{i=1}^{3}\sqrt{1+\frac{7}{9+4^2}}}{\sqrt{1+\frac{3}{1+2^2}}} > 1.$$

Case 2. $u \sim v$.

$$\frac{\prod_{\mathrm{SO}}(T^*)}{\prod_{\mathrm{SO}}(T)} = \frac{\sqrt{1+16}\sqrt{16+d^2(u_1)}\sqrt{16+d^2(v_1)}\sqrt{16+d^2(v_3)}}{\sqrt{4+9}\sqrt{4+d^2(u_1)}\sqrt{9+d^2(v_1)}\sqrt{9+d^2(v_3)}} > 1.$$

As required, we complete the proof. □

Lemma 2.4 ([11]) *Let $T \in \mathcal{CT}_n^*$, and p be the number of pendent vertices in T. Then*

(1) if $n \equiv 0 \pmod 3$, then $n_2 = 1$, $n_3 = 0$ and $p = \frac{2n}{3}$;

(2) if $n \equiv 1 \pmod 3$, then $n_2 = 0$, $n_3 = 1$ and $p = \frac{2n+1}{3}$;

(3) if $n \equiv 2 \pmod 3$, then $n_2 = 0$, $n_3 = 0$ and $p = \frac{2n+2}{3}$.

Theorem 2.5 *Let $T \in \mathcal{CT}_n$, $n \geq 13$. Then*

$$\prod\nolimits_{\mathrm{SO}}(T) \leq \begin{cases} 20 \cdot 17^{\frac{n}{3}} \cdot 32^{\frac{n-9}{6}}, & n \equiv 0 \pmod 3\\ 2125 \cdot 17^{\frac{2n-5}{6}} \cdot 32^{\frac{n-13}{6}}, & n \equiv 1 \pmod 3\\ 17^{\frac{n+1}{3}} \cdot 32^{\frac{n-5}{6}}, & n \equiv 2 \pmod 3). \end{cases}$$

Proof From the Lemmas 2.1–2.3, we know that if $T \in \mathcal{CT}_n$ has maximum multiplicative Sombor index, then $T \in \mathcal{CT}_n^*$. Let p be the number of pendent vertices in T. By Lemma 2.4, we have

Case 1. $n \equiv 0 \pmod 3$, then $n_2 = 1$, $n_3 = 0$ and $p = \frac{2n}{3}$.

Let $d(u) = 2$, $N_T(u) = \{u_1, u_2\}$.

If $d(u_1) = 1$ or $d(u_2) = 1$, then

$$\prod\nolimits_{SO}(T) = \sqrt{1^2+2^2}\cdot\sqrt{2^2+4^2}\cdot(1^2+4^2)^{\frac{p-1}{2}}\cdot(4^2+4^2)^{\frac{n-p-2}{2}}$$
$$=10\cdot 17^{\frac{2n-3}{6}}\cdot 32^{\frac{n-6}{6}} = \frac{40\sqrt{2}}{\sqrt{17}}\cdot 17^{\frac{n}{3}}\cdot 32^{\frac{n-9}{6}}.$$

If $d(u_1) = d(u_2) = 4$, then

$$\prod\nolimits_{SO}(T) = (2^2+4^2)\cdot(1^2+4^2)^{\frac{p}{2}}\cdot(4^2+4^2)^{\frac{n-p-3}{2}} = 20\cdot 17^{\frac{n}{3}}\cdot 32^{\frac{n-9}{6}}.$$

Case 2. $n \equiv 1 \pmod 3$, then $n_2 = 0$, $n_3 = 1$ and $p = \frac{2n+1}{3}$.

Let $d(v) = 3$, $N_T(v) = \{v_1, v_2, v_3\}$. Suppose that $d(v_1) \le d(v_2) \le d(v_3)$.

If $d(v_1) = 1$ and $d(v_2) = d(v_3) = 4$, then

$$\prod\nolimits_{SO}(T) = \sqrt{1^2+3^2}\cdot(3^2+4^2)\cdot(1^2+4^2)^{\frac{p-1}{2}}\cdot(4^2+4^2)^{\frac{n-p-3}{2}}$$
$$=25\sqrt{10}\cdot 17^{\frac{n-1}{3}}\cdot 32^{\frac{n-10}{6}} = 25\sqrt{5440}\cdot 17^{\frac{2n-5}{6}}\cdot 32^{\frac{n-13}{6}}.$$

If $d(v_1) = d(v_2) = 1$ and $d(v_3) = 4$, then

$$\prod\nolimits_{SO}(T) = (1^2+3^2)\cdot\sqrt{3^2+4^2}\cdot(1^2+4^2)^{\frac{p-2}{2}}\cdot(4^2+4^2)^{\frac{n-p-2}{2}}$$
$$=50\cdot 17^{\frac{2n-5}{6}}\cdot 32^{\frac{n-7}{6}} = 1600\cdot 17^{\frac{2n-5}{6}}\cdot 32^{\frac{n-13}{6}}.$$

If $d(v_1) = d(v_2) = d(v_3) = 4$, then

$$\prod\nolimits_{SO}(T) = (3^2+4^2)^{\frac{3}{2}}\cdot(1^2+4^2)^{\frac{p}{2}}\cdot(4^2+4^2)^{\frac{n-p-4}{2}}$$
$$=125\cdot 17^{\frac{2n+1}{6}}\cdot 32^{\frac{n-13}{6}} = 2125\cdot 17^{\frac{2n-5}{6}}\cdot 32^{\frac{n-13}{6}}.$$

Case 3. $n \equiv 2 \pmod 3$, then $n_2 = 0$, $n_3 = 0$ and $p = \frac{2n+2}{3}$

$$\prod\nolimits_{SO}(T) = (1^2+4^2)^{\frac{p}{2}}\cdot(4^2+4^2)^{\frac{n-p-1}{2}} 17^{\frac{n+1}{3}}\cdot 32^{\frac{n-5}{6}}.$$

This completes the proof. □

3. The first thirteen minimum (molecular) trees

Denote by $\mathcal{T}$ (resp., $\mathcal{T}_n$) the set of trees (resp., trees with n vertices). We first introduce some important transformations which will decrease the multiplicative Sombor index.

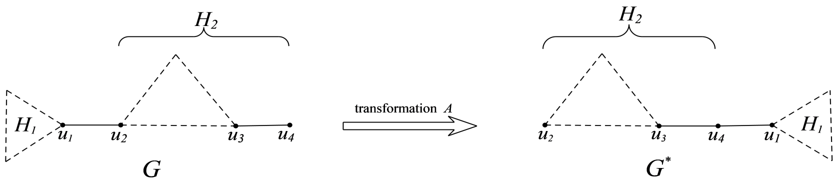

Figure 1 Transformation A of Lemma 3.1

Lemma 3.1 *Let $H_1, H_2 \in \mathcal{T}$ and $u_1 \in V(H_1)$, $\{u_2, u_3, u_4\} \subseteq V(H_2)$, $u_3u_4 \in E(H_2)$. $d_{H_2}(u_2) \triangleq t \ge 3$, $d_{H_2}(u_3) \triangleq z \ge 2$, $d_{H_2}(u_4) = 1$, and $t \triangleq d_{H_2}(u_2) \ge d_{H_1}(u_1) \triangleq y$. Suppose that G is the* *graph obtained from H_1 and H_2 by connecting vertices u_1 and u_2. Let $G^* = G - \{u_1u_2\} + \{u_1u_4\}$ (see Figure 1). Then $\prod_{\rm SO}(G^*) < \prod_{\rm SO}(G)$.*

Proof Let $N_{H_2}(u_2) = \{w_1, w_2, \ldots, w_t\}$, $d_{H_2}(w_i) = x_i$ for $i = 1, 2, \ldots, t$.

Case 1. $u_2 \neq u_3$

$$\frac{\prod_{\rm SO}(G)}{\prod_{\rm SO}(G^*)} = \frac{\sqrt{(y+1)^2+(t+1)^2}\cdot\sqrt{(z+1)^2+1}\cdot\prod\_i=1^t\sqrt{x_i^2+(t+1)^2}}{\sqrt{(y+1)^2+4}\cdot\sqrt{z^2+4}\cdot\prod_{i=1}^{t}\sqrt{x_i^2+t^2}} > \frac{\sqrt{(y+1)^2+(t+1)^2}}{\sqrt{(y+1)^2+4}\sqrt{1+\frac{3}{1+z^2}}}.$$

Since $z \geq 2$, $t \geq 3$, $t \geq y$, we have

If $y \geq 3$, then

$$\frac{\prod_{\rm SO}(G)}{\prod_{\rm SO}(G^*)} > \frac{\sqrt{(y+1)^2+(t+1)^2}}{\sqrt{\frac{8}{5}}\cdot\sqrt{(y+1)^2+4}} \geq \frac{\sqrt{2(y+1)^2}}{\sqrt{\frac{8}{5}}\cdot\sqrt{(y+1)^2+4}} > 1.$$

If $y = 2$, then

$$\frac{\prod_{\rm SO}(G)}{\prod_{\rm SO}(G^*)} > \frac{\sqrt{9+(t+1)^2}}{\sqrt{\frac{8}{5}}\cdot\sqrt{13}} \geq \frac{\sqrt{9+4^2}}{\sqrt{\frac{8}{5}}\cdot\sqrt{13}} > 1.$$

If $y = 1$, then

$$\frac{\prod_{\rm SO}(G)}{\prod_{\rm SO}(G^*)} > \frac{\sqrt{4+(t+1)^2}}{\sqrt{\frac{8}{5}}\cdot\sqrt{8}} \geq \frac{\sqrt{4+4^2}}{\sqrt{\frac{8}{5}}\cdot\sqrt{8}} > 1.$$

Case 2. $u_2 \equiv u_3$.

In this case, we suppose $w_1 \equiv u_4$. Then

$$\frac{\prod_{\rm SO}(G)}{\prod_{\rm SO}(G^*)} = \frac{\sqrt{(y+1)^2+(t+1)^2}\cdot\sqrt{(t+1)^2+1}\cdot\prod_{i=2}^{t}\sqrt{x_i^2+(t+1)^2}}{\sqrt{(y+1)^2+4}\cdot\sqrt{t^2+4}\cdot\prod_{i=2}^{t}\sqrt{x_i^2+t^2}} > 1.$$

As required, we complete the proof. □

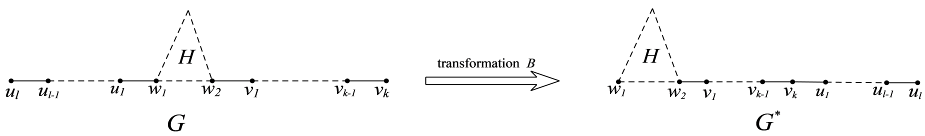

Figure 2 Transformation B of Lemma 3.2

Lemma 3.2 *Let $H \in \mathcal{T}$ and $w_1, w_2 \in V(H)$, $d_H(w_1) \geq 2$, and $P_1 = u_1u_2\cdots u_l$, $P_2 = v_1v_2\cdots v_k$ are two paths. Suppose that G is the graph obtained from H, P_1 and P_2 by adding edge u_1w_1 and w_2v_1. Let $G^* = G - \{u_1w_1\} + \{u_1v_k\}$ (see Figure 2). Then $\prod_{\rm SO}(G^*) < \prod_{\rm SO}(G)$.*

Proof If $d_H(w_1) \geq 3$, by transformation A of Lemma 3.1, the conclusion holds. Next we only consider $d_H(w_1) = 2$. Let $d_H(w_1) = 2$, $N_H(w_1) = \{x_1, x_2\}$, $d_H(x_i) = d_i$ $(i = 1, 2)$.

If $w_1 \neq w_2$, $k, l \geq 2$.

$$\frac{\prod_{\rm SO}(G)}{\prod_{\rm SO}(G^*)} = \frac{\sqrt{2^2+3^2}\cdot\sqrt{2^2+1^2}\cdot\prod_{i=1}^{2}\sqrt{d_i^2+3^2}}{\sqrt{2^2+2^2}\cdot\sqrt{2^2+2^2}\cdot\prod_{i=1}^{2}\sqrt{d_i^2+2^2}} > 1.$$

If $w_1 \neq w_2$, $k=1$, $l \geq 2$. Let $d_G(w_2)=t$. Then

$$\frac{\prod_{\mathrm{SO}}(G)}{\prod_{\mathrm{SO}}(G^*)} = \frac{\sqrt{2^2+3^2}\cdot\sqrt{t^2+1^2}\cdot\prod_{i=1}^{2}\sqrt{d_i^2+3^2}}{\sqrt{2^2+2^2}\cdot\sqrt{2^2+t^2}\cdot\prod_{i=1}^{2}\sqrt{d_i^2+2^2}}.$$

Since $t \geq 2$,

$$\begin{aligned}&13(t^2+1)(d_1^2+9)(d_2^2+9)-8(t^2+4)(d_1^2+4)(d_1^2+4)\\ &=[5d_1^2d_2^2+85d_1^2+85d_2^2+925]t^2-19d_1^2d_2^2-11d_1^2-11d_2^2+541>0.\end{aligned}$$

Thus, $\frac{\prod_{\mathrm{SO}}(G)}{\prod_{\mathrm{SO}}(G^*)}>1$.

If $w_1 \neq w_2$, $k=1, k \geq 2$.

$$\frac{\prod_{\mathrm{SO}}(G)}{\prod_{\mathrm{SO}}(G^*)} = \frac{\sqrt{1^2+3^2}\cdot\prod_{i=1}^{2}\sqrt{d_i^2+3^2}}{\sqrt{2^2+2^2}\cdot\prod_{i=1}^{2}\sqrt{d_i^2+2^2}}>1.$$

If $w_1 \neq w_2$, $k=1, l=1$. Let $d_G(w_2)=t$. Since $t \geq 2$, we have

$$\begin{aligned}\frac{\prod_{\mathrm{SO}}(G)}{\prod_{\mathrm{SO}}(G^*)} &= \frac{\sqrt{1^2+3^2}\cdot\sqrt{t^2+1^2}\cdot\prod_{i=1}^{2}\sqrt{d_i^2+3^2}}{\sqrt{1^2+2^2}\cdot\sqrt{2^2+t^2}\cdot\prod_{i=1}^{2}\sqrt{d_i^2+2^2}}\\ &=\frac{\sqrt{2}\prod\limits_{i=1}^{2}\sqrt{1+\frac{5}{4+d_i^2}}}{\sqrt{1+\frac{5}{4+t^2}}} \geq \frac{4}{\sqrt{11}}\prod_{i=1}^{2}\sqrt{1+\frac{5}{4+d_i^2}}>1.\end{aligned}$$

If (1) $w_1=w_2$, $k,l \geq 2$, (2)$w_1=w_2$, $k=1, l\geq 2$, (3) $w_1=w_2$, $l=1, k\geq 2$, (4) $w_1=w_2$, $l=1, k=1$, we can similarly proof. □

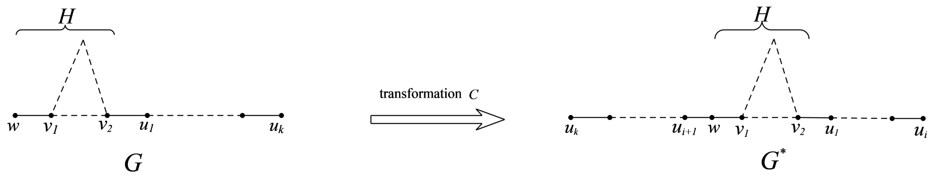

Figure 3 Transformation C of Lemma 3.3

Lemma 3.3 *Let $H \in \mathcal{T}$ and $v_1, v_2, w \in V(H)$, $d_H(v_1) \triangleq t \geq 3$, $d_H(v_2) \geq 2$, $d_H(w)=1$ and $P_1=u_1u_2\cdots u_k$ be a path. Suppose that G is the graph obtained from H and P by adding edge v_2u_1. Let $G^*=G-\{u_iu_{i+1}\}+\{u_{i+1}w\}$ $(2 \leq i \leq k-1)$ (see Figure 3). Then $\prod_{\mathrm{SO}}(G^*)<\prod_{\mathrm{SO}}(G)$.*

Proof Since $t \geq 3$, if $v_1 \neq v_2$, then

$$\frac{\prod_{\mathrm{SO}}(G)}{\prod_{\mathrm{SO}}(G^*)} = \frac{\sqrt{2^2+2^2}\sqrt{1^2+t^2}}{\sqrt{1^2+2^2}\cdot\sqrt{2^2+t^2}} = \frac{\sqrt{\frac{8}{5}}}{\sqrt{1+\frac{3}{1+t^2}}}>1.$$

If $v_1=v_2$, then

$$\frac{\prod_{\mathrm{SO}}(G)}{\prod_{\mathrm{SO}}(G^*)} = \frac{\sqrt{2^2+2^2}\sqrt{1^2+(t+1)^2}}{\sqrt{1^2+2^2}\cdot\sqrt{2^2+(t+1)^2}} = \frac{\sqrt{\frac{8}{5}}}{\sqrt{1+\frac{3}{1+(t+1)^2}}}>1.$$

As required, we complete the proof. □

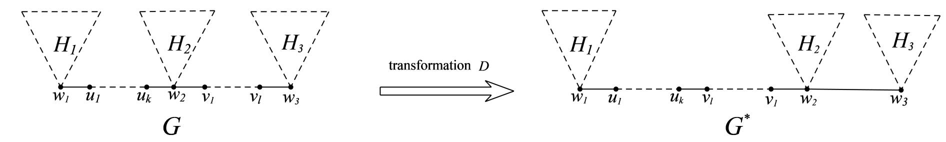

Figure 4 Transformation D of Lemma 3.4

Lemma 3.4 *Let $H_i \in \mathcal{T}$ and $w_i \in V(H_i)$ $(i=1,2,3)$, $d_{H_3}(w_3) \triangleq x \ge 2$, $d_{H_2}(w_2) \triangleq y \ge 1$, $d_{H_1}(w_1) \ge 1$ and $P_1 = u_1u_2\cdots u_k$, $P_2 = v_1v_2\cdots v_l$ be two paths. Suppose that G is the graph obtained from H_1, H_2, H_3, P_1, P_2 by adding edges w_1u_1, u_kw_2, w_2v_1, v_lw_3. Let $G^* = G - \{u_kw_2, v_lw_3\} + \{u_kv_l, w_2w_3\}$ (see Figure 4). Then $\prod_{\rm SO}(G^*) < \prod_{\rm SO}(G)$.*

Proof We know that

$$\frac{\prod_{\rm SO}(G)}{\prod_{\rm SO}(G^*)} = \frac{\sqrt{(y+2)^2+2^2}\sqrt{(x+1)^2+2^2}}{\sqrt{2^2+2^2}\sqrt{(x+1)^2+(y+2)^2}}.$$

Since $x \ge 2$, $y \ge 1$, we have $[(y+2)^2+4][(x+1)^2+4] - 8[(x+1)^2+(y+2)^2] = [(y+2)^2-4](x+1)^2 - 4(y+2)^2 + 16 \ge 9[(y+2)^2-4] - 4(y+2)^2 + 16 > 0$, thus $\frac{\prod_{\rm SO}(G)}{\prod_{\rm SO}(G^*)} > 1$. As required, the proof is completed. □

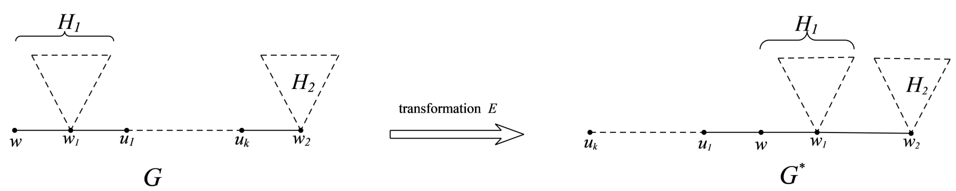

Figure 5 Transformation E of Lemma 3.5

Lemma 3.5 *Let $H_1, H_2 \in \mathcal{T}$ and $\{w, w_1\} \subseteq V(H_1)$, $ww_1 \in E(H_1)$, $w_2 \in V(H_2)$, $d_{H_1}(w_1) \triangleq x \ge 2$, $d_{H_2}(w_2) \triangleq y \ge 2$, $ww_1 \in E(H_1)$, $d_{H_1}(w) = 1$ and $P = u_1u_2\cdots u_k$ be a path. Suppose that G is the graph obtained from H_1, H_2, P by adding edges w_1u_1, u_kw_2. Let $G^* = G - \{w_1u_1, u_kw_2\} + \{w_1w_2, u_1w\}$ (see Figure 5). Then $\prod_{\rm SO}(G^*) < \prod_{\rm SO}(G)$.*

Proof We know that

$$\frac{\prod_{\rm SO}(G)}{\prod_{\rm SO}(G^*)} = \frac{\sqrt{(x+1)^2+1^2}\sqrt{(y+1)^2+2^2}}{\sqrt{1^2+2^2}\sqrt{(x+1)^2+(y+1)^2}}.$$

Since $x \ge 2$, $y \ge 2$, if $x \ge y$, then

$$\begin{aligned}&[(x+1)^2+1][(y+1)^2+4] - 5[(x+1)^2+(y+1)^2]\\ &\quad = (x+1)^2(y+1)^2 - (x+1)^2 - 4(y+1)^2 + 4 \ge 4(x+1)^2 + 4 > 0.\end{aligned}$$

If $x \le y$, then

$$[(x+1)^2+1][(y+1)^2+4] - 5[(x+1)^2+(y+1)^2]$$

$$= (x+1)^2(y+1)^2 - (x+1)^2 - 4(y+1)^2 + 4 \geq 4(y+1)^2 + 4 > 0,$$

thus $\frac{\prod_{\mathrm{SO}}(G)}{\prod_{\mathrm{SO}}(G^*)} > 1$.

As required, we complete the proof. □

Denote by $T_n(a_1, a_2, \ldots, a_m)$ the starlike tree with n vertices obtained from star S_{m+1} by replacing its m edges by m paths $P_{a_1}, P_{a_2}, \ldots, P_{a_m}$ and $\sum_{i=1}^m a_i + 1 = n$. Let $T \in \mathcal{T}_n$ have two branching vertices u_1, u_2, and $d_T(u_1) = k$, $d_T(u_2) = l$. Suppose that the $k-1$ components of $T - u_1$ are $p_1, p_2, \ldots, p_{k-1}$, the $l-1$ components of $T - u_2$ are $q_1, q_2, \ldots, q_{l-1}$, then we write $T = T_n(p_1, p_2, \ldots, p_{k-1}; q_1, q_2, \ldots, q_{l-1})$. If $u_1 \sim u_2$, then we write $T = T_n^{\sim}(p_1, p_2, \ldots, p_{k-1}; q_1, q_2, \ldots, q_{l-1})$. If $u_1 \nsim u_2$, then we write $T = T_n^{\nsim}(p_1, p_2, \ldots, p_{k-1}; q_1, q_2, \ldots, q_{l-1})$.

Denote by $T(a_1^{(b_1)}, a_2^{(b_2)}, \ldots, a_m^{(b_m)})$ the degree sequences of T, i.e., the set of trees with b_i vertices of degree a_i $(i = 1, 2, \ldots, m)$. Denote by $A(n) = \{T \in T(3^{(3)}, 2^{(n-8)}, 1^{(5)}) | m_{1,2}(T) = 5, m_{2,3}(T) = 5, m_{3,3}(T) = 2, m_{2,2}(T) = n - 13\}$ $(n \geq 13)$.

Theorem 3.6 *Let $T \in \mathcal{T}_n$ $(n \geq 13)$, $\Delta(T) \geq 4$ and $T \notin T_n(a_1, a_2, a_3, a_4)$ $(a_i \geq 2, i = 1, 2, 3, 4)$. Then for $T^* \in T_n(a_1, a_2, a_3, a_4)$ $(a_i \geq 2, i = 1, 2, 3, 4)$, we have $\prod_{\mathrm{SO}}(T^*) < \prod_{\mathrm{SO}}(T)$.*

Proof We consider the following two cases.

Case 1. $\Delta(T) = 4$.

Subcase 1.1. $T \in T(4^{(1)}, 2^{(n-5)}, 1^{(4)})$ and there exists $i \in \{1, 2, 3, 4\}$, such that $a_i = 1$.

Using Transformation C of Lemma 3.3, we can obtain a tree T', such that the paths P_i with $a_i \geq 2$ are more and more, and the paths P_j with $a_j = 1$ are less and less, and $\prod_{\mathrm{SO}}(T') < \prod_{\mathrm{SO}}(T)$. Using Transformation C repeatedly, we can obtain $T^* \in T_n(a_1, a_2, a_3, a_4)$ $(a_i \geq 2, i = 1, 2, 3, 4)$ and $\prod_{\mathrm{SO}}(T^*) < \prod_{\mathrm{SO}}(T)$.

Subcase 1.2. $T \notin T(4^{(1)}, 2^{(n-5)}, 1^{(4)})$.

Using Transformation B of Lemma 3.2, repeatedly, we can obtain a tree $T'' \in T(4^{(1)}, 2^{(n-5)}, 1^{(4)})$ and $\prod_{\mathrm{SO}}(T'') < \prod_{\mathrm{SO}}(T)$. Then by Subcase 1.1, we can obtain $T^* \in T_n(a_1, a_2, a_3, a_4)$ $(a_i \geq 2, i = 1, 2, 3, 4)$ and $\prod_{\mathrm{SO}}(T^*) < \prod_{\mathrm{SO}}(T)$.

Case 2. $\Delta(T) \geq 5$.

By Transformation A of Lemma 3.1, repeatedly, we can obtain a tree T' such that $\Delta(T') = 4$ and $\prod_{\mathrm{SO}}(T') < \prod_{\mathrm{SO}}(T)$. Then by Case 1, we can obtain $T^* \in T_n(a_1, a_2, a_3, a_4)$ $(a_i \geq 2, i = 1, 2, 3, 4)$ and $\prod_{\mathrm{SO}}(T^*) < \prod_{\mathrm{SO}}(T)$. □

Theorem 3.7 *Let $T \in \mathcal{T}_n$ $(n \geq 13)$, $\Delta(T) = 3$, $n_3(T) \geq 3$ and $T \notin A(n)$. Then for $T^* \in A(n)$, we have $\prod_{\mathrm{SO}}(T^*) < \prod_{\mathrm{SO}}(T)$.*

Proof We consider the following two cases.

Case 1. $n_3(T) = 3$.

Since $n_3(T) = 3$ and $T \notin A(n)$, then $m_{1,2}(T) \neq 5$ $(m_{2,3}(T) \neq 5)$, $m_{3,3}(T) = 2$, or $m_{1,2}(T) = 5$ $(m_{2,3}(T) = 5)$, $m_{3,3}(T) \neq 2$, or $m_{1,2}(T) \neq 5$ $(m_{2,3}(T) \neq 5)$, $m_{3,3}(T) \neq 2$.

Subcase 1.1. $m_{1,2}(T) \neq 5$ $(m_{2,3}(T) \neq 5)$, $m_{3,3}(T) = 2$.

Using Transformation C of Lemma 3.3, repeatedly, we can obtain $T^* \in A(n)$ and $\prod_{\mathrm{SO}}(T^*) < \prod_{\mathrm{SO}}(T)$.

Subcase 1.2. $m_{1,2}(T) = 5$ $(m_{2,3}(T) = 5)$, $m_{3,3}(T) \neq 2$.

Using Transformation D and E of Lemmas 3.4 and 3.5, repeatedly, we can obtain $T^* \in A(n)$ and $\prod_{\mathrm{SO}}(T^*) < \prod_{\mathrm{SO}}(T)$.

Subcase 1.2. $m_{1,2}(T) \neq 5$ $(m_{2,3}(T) \neq 5)$, $m_{3,3}(T) \neq 2$.

Using Transformation D and E of Lemmas 3.4 and 3.5, repeatedly, we can obtain T' such that $m_{3,3}(T') = 2$. Then using Transformation C of Lemma 3.3, repeatedly, we can obtain $T^* \in A(n)$ and $\prod_{\mathrm{SO}}(T^*) < \prod_{\mathrm{SO}}(T)$.

Case 2. $n_3(T) \geq 4$.

Using Transformation B of Lemma 3.2, repeatedly, we can obtain T' such that $n_3(T') = 3$. Then by Case 1, we can obtain $T^* \in A(n)$ and $\prod_{\mathrm{SO}}(T^*) < \prod_{\mathrm{SO}}(T)$. □

If $G \in T(a_1, a_2, a_3, a_4)$ $(a_i \geq 2, i = 1, 2, 3, 4)$, then $\prod_{\mathrm{SO}}(G) = 10000 \cdot 8^{\frac{n-9}{2}}$. If $G \in A(n)$, then $\prod_{\mathrm{SO}}(G) = 18 \cdot (65)^{\frac{5}{2}} \cdot 8^{\frac{n-13}{2}}$. By Theorems 3.6, 3.7 and Table 1, we determine the first thirteen minimum tree with respect to multiplicative Sombor index.

Number	Notation	$\prod_{\mathrm{SO}}$
(1)	P_n	$5 \cdot 8^{\frac{n-3}{2}}$
(2)	$T_n(a_1, a_2, a_3)$	$(65)^{\frac{3}{2}} \cdot 8^{\frac{n-7}{2}}$
(3)	$T_n(a_1, a_2, 1)$	$65 \cdot (10)^{\frac{1}{2}} \cdot 8^{\frac{n-6}{2}}$
(4)	$T_n(a_1, 1, 1)$	$10 \cdot (65)^{\frac{1}{2}} \cdot 8^{\frac{n-5}{2}}$
(5)	$T_n^{\sim}(p_{a_1}, p_{a_2}; q_{b_1}, q_{b_2})$	$17925 \cdot 8^{\frac{n-10}{2}}$
(6)	$T_n^{\nsim}(p_{a_1}, p_{a_2}; q_{b_1}, q_{b_2})$	$54925 \cdot 8^{\frac{n-11}{2}}$
(7)	$T_n^{\sim}(p_{a_1}, p_{a_2}; q_{b_1}, 1)$	$(180)^{\frac{1}{2}} \cdot (65)^{\frac{3}{2}} \cdot 8^{\frac{n-9}{2}}$
(8)	$T_n^{\nsim}(p_{a_1}, p_{a_2}; q_{b_1}, 1)$	$(10)^{\frac{1}{2}} \cdot (5)^{\frac{3}{2}} \cdot (13)^{\frac{5}{2}} \cdot 8^{\frac{n-10}{2}}$
(9)	$T_n^{\sim}(p_{a_1}, 1; q_{b_1}, 1)$ or $T_n^{\sim}(p_{a_1}, p_{a_2}; 1, 1)$	$650 \cdot (18)^{\frac{1}{2}} \cdot 8^{\frac{n-8}{2}}$
(10)	$T_n^{\nsim}(p_{a_1}, 1; q_{b_1}, 1)$ or $T_n^{\nsim}(p_{a_1}, p_{a_2}; 1, 1)$	$8450 \cdot 8^{\frac{n-9}{2}}$
(11)	$T_n^{\sim}(p_{a_1}, 1; 1, 1)$	$(1170)^{\frac{1}{2}} \cdot (10)^{\frac{3}{2}} \cdot 8^{\frac{n-7}{2}}$
(12)	$T_n^{\nsim}(p_{a_1}, 1; 1, 1)$	$(5)^{\frac{1}{2}} \cdot (130)^{\frac{3}{2}} \cdot 8^{\frac{n-8}{2}}$
(13)	$T_n^{\nsim}(1, 1; 1, 1)$	$1300 \cdot 8^{\frac{n-7}{2}}$

Table 1 Tree $T \in T_n$ with $\Delta(T) \leq 3$, $n_3(T) \leq 2$ $(a_i, b_i \geq 2)$ and their $\prod_{\mathrm{SO}}$

Theorem 3.8 *Let* $G \in \mathcal{T}_n$ $(n \geq 13)$, $T_1 = P_n$, $T_2 \in T_n(a_1, a_2, a_3)$, $T_3 \in T_n(a_1, a_2, 1)$, $T_4 \in T_n(a_1, 1, 1)$, $T_5 \in T_n^{\sim}(p_{a_1}, p_{a_2}; q_{b_1}, q_{b_2})$, $T_6 \in T_n^{\nsim}(p_{a_1}, p_{a_2}; q_{b_1}, q_{b_2})$, $T_7 \in T_n^{\sim}(p_{a_1}, p_{a_2}; q_{b_1}, 1)$, $T_8 \in T_n^{\nsim}(p_{a_1}, p_{a_2}; q_{b_1}, 1)$, $T_9 \in T_n^{\sim}(p_{a_1}, 1; q_{b_1}, 1)$ *or* $T_9 \in T_n^{\sim}(p_{a_1}, p_{a_2}; 1, 1)$, $T_{10} \in T_n^{\nsim}(p_{a_1}, 1; q_{b_1}, 1)$ *or* $T_{10} \in T_n^{\nsim}(p_{a_1}, p_{a_2}; 1, 1)$, $T_{11} \in T_n^{\sim}(p_{a_1}, 1; 1, 1)$, $T_{12} \in T_n^{\nsim}(p_{a_1}, 1; 1, 1)$, $T_{13} \in A(n)$. *If* $G \notin \{T_1, T_2, \ldots, T_{13}\}$, *then* $\prod_{\mathrm{SO}}(T_1) < \prod_{\mathrm{SO}}(T_2) < \cdots < \prod_{\mathrm{SO}}(T_{13}) < \prod_{\mathrm{SO}}(G)$.

Denote by $\mathcal{CT}_n$ the set of molecular trees with n vertices. Since the first thirteen minimum trees are also molecular trees, thus we have

Theorem 3.9 *Let* $G \in \mathcal{CT}_n$ $(n \geq 13)$, $T_1 = P_n$, $T_2 \in T_n(a_1, a_2, a_3)$, $T_3 \in T_n(a_1, a_2, 1)$, $T_4 \in T_n(a_1, 1, 1)$, $T_5 \in T_n^{\sim}(p_{a_1}, p_{a_2}; q_{b_1}, q_{b_2})$, $T_6 \in T_n^{\approx}(p_{a_1}, p_{a_2}; q_{b_1}, q_{b_2})$, $T_7 \in T_n^{\sim}(p_{a_1}, p_{a_2}; q_{b_1}, 1)$, $T_8 \in T_n^{\approx}(p_{a_1}, p_{a_2}; q_{b_1}, 1)$, $T_9 \in T_n^{\sim}(p_{a_1}, 1; q_{b_1}, 1)$ *or* $T_9 \in T_n^{\sim}(p_{a_1}, p_{a_2}; 1, 1)$, $T_{10} \in T_n^{\approx}(p_{a_1}, 1; q_{b_1}, 1)$ *or* $T_{10} \in T_n^{\approx}(p_{a_1}, p_{a_2}; 1, 1)$, $T_{11} \in T_n^{\sim}(p_{a_1}, 1; 1, 1)$, $T_{12} \in T_n^{\approx}(p_{a_1}, 1; 1, 1)$, $T_{13} \in A(n)$. *If* $G \notin \{T_1, T_2, \ldots, T_{13}\}$, *then* $\prod_{\mathrm{SO}}(T_1) < \prod_{\mathrm{SO}}(T_2) < \cdots < \prod_{\mathrm{SO}}(T_{13}) < \prod_{\mathrm{SO}}(G)$.

Analogous results also hold for the multiplicative reduced Sombor index, in which $d(u)$ is replaced by $d(u) - 1$.

4. Concluding remarks

In this paper, we determine the maximum molecular trees and the first thirteen minimum (molecular) trees with respect to the multiplicative Sombor index. On the one hand, one can further order trees with respect to the multiplicative Sombor index. On the other hand, one can determine the extremal multiplicative Sombor index of other classes of graphs.

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