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The Sombor index and harmonic index of chemical trees with a given number of vertices of maximum degree

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Abstract

For a graph G, the Sombor index and harmonic index are respectively defined as

$$SO(G) = \sum_{uv\in E(G)} \sqrt{deg_G^2(u) + deg_G^2(v)} \quad \text{and} \quad \mathcal{H}(G) = \sum_{uv\in E(G)} \frac{2}{deg_G(u)+deg_G(v)},$$

where $E(G)$ is the edge set and $deg_G(u)$ denoting the degree of a vertex u in G. In this paper, we aim to find extremal trees in the class of chemical trees with the given number of vertices of degree 4 for the Sombor index and the harmonic index. We observe that the extremal chemical trees maximizing the Sombor index also minimize the harmonic index in this class. Furthermore, we construct the corresponding extremal trees.

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1. Introduction

Let $G = (V(G), E(G))$ be a simple graph with order n and size m, where $V(G)$ and $E(G)$ denote its vertex set and edge set, respectively. The degree of a vertex u is denoted by $deg_G(u)$. A path is a sequence of distinct vertices $v_1, v_2, v_3, \dots, v_n$, in which two vertices are adjacent if they are consecutive in the

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sequence. A tree with each vertex having its degree less than or equal to 4 is called a chemical tree. The graph $G - uv$ is obtained by removing the edge uv, and $G + uv$ is derived by inserting an edge between the vertices u and v that are non-adjacent. Denote by S_n the star graph with order n. The double star graph $S_{p,q}$ is a tree with exactly two non-pendant vertices that are adjacent by an edge, one with degree p and other with degree q. The number of edges between vertices of degree i and j is denoted by $m_{ij}(G)$, and $n_i(G)$ represents the the number of vertices with degree i.

The topological indices are used to analyze molecular structure graphs and characterize the physicochemical properties of a compound. Harry Wiener presented the Wiener index to examine the boiling points of alkanes [1]. In literature, several vertex-degree-based topological indices have been introduced and extensively studied [2]. Fajtlowicz [3] defined the harmonic index as part of certain conjectures generated by the computer program Graffiti and defined it as

$$\mathcal{H}(G) = \sum_{uv\in E(G)} \frac{2}{deg_G(u)+deg_G(v)}.$$

After [4], the harmonic index gained substantial attention, which led to numerous publications, and research is still ongoing on this index [5-7].

In 2021, Gutman [8] introduced the Sombor index using the geometric framework and expressed it as

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

This geometric perspective on the Sombor index has quickly captured the interest of researchers [9-12]. Extremal (chemical) trees are found under various degree parameters for the Sombor index and harmonic index [9, 11, 13-21]. For other indices, several results on extremal graphs have been documented in the literature [22-24]. Finding extremal trees is a key problem in chemical graph theory. Zhou, Lin, and Miao [25] determined the maximum Sombor index among trees and unicyclic graphs with a fixed matching number. Since vertex degree corresponds to molecular bonds, addressing problems under specific degree constraints is important. In this context, we find extremal chemical trees with k vertices of 4 degree for the SO and H indices. In [14], the authors provide the following relationships for a chemical tree:

$$2m_{11}(G) + m_{12}(G) + m_{13}(G) + m_{14}(G) = n_1(G), \quad (1.1)$$

$$m_{12}(G) + 2m_{22}(G) + m_{23}(G) + m_{24}(G) = 2n_2(G), \quad (1.2)$$

$$m_{13}(G) + m_{23}(G) + 2m_{33}(G) + m_{34}(G) = 3n_3(G), \quad (1.3)$$

$$m_{14}(G) + m_{24}(G) + m_{34}(G) + 2m_{44}(G) = 4n_4(G). \quad (1.4)$$

Clearly

$$n(G) = n_1(G) + n_2(G) + n_3(G) + n_4(G). \quad (1.5)$$

By the handshaking lemma, the following holds:

$$2(n(G) - 1) = n_1(G) + 2n_2(G) + 3n_3(G) + 4n_4(G). \quad (1.6)$$

The Sombor index and harmonic index of a chemical tree can be restated as follows, respectively:

$$SO(T) = \sum_{1\le i\le j\le 4} \sqrt{i^2+j^2}\, m_{ij}(T), \tag{1.7}$$

$$\mathcal{H}(T) = \sum_{1\le i\le j\le 4} \frac{2}{i+j} m_{ij}(T). \tag{1.8}$$

Let $\mathcal{CT}_{n,k}$ be the set of chemical trees of given order $n\ (\ge 3k+2)$ with exactly $k \ge 1$ vertices of degree 4. A chemical tree in $\mathcal{CT}_{n,k}$ is graphically feasible for $n \ge 3k+2$. For each $n \in \{5,6\}$ and $k=1$, $\mathcal{CT}_{n,k}$ has only one chemical tree, namely, S_5 and $S_{4,2}$. For different brackets of n and k, the extremal trees in the class $\mathcal{CT}_{n,k}$ are different. This motivates us to define the following sub-classes:

$\mathcal{C}_1\mathcal{T}_{n,k} = \{T \in \mathcal{CT}_{n,k} | 3k+2 \le n \le 4k, k \ge 2\}$,
$\mathcal{C}_2\mathcal{T}_{n,k} = \{T \in \mathcal{CT}_{n,k} | 4k < n < 5k-2, k \ge 4\} \cup \{T \in \mathcal{CT}_{n,k} | n = 9, k = 2\}$,
$\mathcal{C}_3\mathcal{T}_{n,k} = \{T \in \mathcal{CT}_{n,k} | n \ge 5k-2, k \ge 3\} \cup \{T \in \mathcal{CT}_{n,k} | n \ge 3k+4, k \in \{1,2\}\}$.

In this paper, we aim to find extremal chemical trees in $\mathcal{CT}_{n,k}$ for SO index and H index. These extremal chemical trees maximizing the SO index also minimize the H index. Furthermore, we construct the corresponding extremal trees.

2. Chemical trees with maximum SO index and minimum H index

In this section, we present the extremal trees that exhibit the maximum SO index value and minimum H index value in the class $\mathcal{CT}_{n,k}$. To prove the main theorem, we need the following results:

Lemma 2.1: *If* $x \ge 0$, $a > b > 0$, *and* $c \ge 1$, *then*

(i) $\sqrt{x^2+a} - \sqrt{x^2+b} > 0$.
(ii) $\frac{c}{x+a} - \frac{c}{x+b} < 0$.
(iii) $h(x) = \sqrt{x^2+b} - \sqrt{x^2+a}$ is strictly increasing.
(iv) $g(x) = \sqrt{x^2+a} - \sqrt{x^2+b}$ is strictly decreasing.
(v) $\Phi(x) = \frac{c}{x+b} - \frac{c}{x+a}$ is strictly decreasing.
(vi) $\Psi(x) = \frac{c}{x+b} - \frac{c}{x+a}$ is strictly increasing.

The following corollary is an immediate result of the handshaking lemma.

Corollary 2.2: [26] *Every graph has an even number of vertices of odd degree.*

In the forthcoming lemmas, we determine the values of m_{ij} and n_i.

Lemma 2.3: *If* $T \in \mathcal{CT}_{n,k}$ *maximizes the Sombor index (minimizes the harmonic index), then* $n_2(T) \le 1$.

Proof: On the contrary, suppose that $n_2(T) > 1$. Then there exist u and v with $deg_T(u) = deg_T(v) = 2$. Now, distinguish the following cases:

Case 1: When $uv \in E(T)$.

Suppose that $u_1 \neq v$ and $v_1 \neq u$ are the neighbor of u and v, respectively. Construct a tree $T' \in \mathcal{CT}_{n,k}$ as follows: $T' = T - uu_1 + vu_1$. Clearly, $deg_{T'}(u) = 1$, $deg_{T'}(v) = 3$ and $deg_{T'}(w) = deg_T(w)$ for all $w \in V(T)\backslash\{u, v\}$. Then

$$\begin{aligned} SO(T') - SO(T) &= \sqrt{deg_T^2(u_1) + 9} - \sqrt{deg_T^2(u_1) + 4} + \sqrt{9 + deg_T^2(v_1)} \\ &\quad - \sqrt{4 + deg_T^2(v_1)} + \sqrt{9 + 1} - \sqrt{4 + 4}. \end{aligned}$$

From Lemma 2.1 (i), we get

$$SO(T') - SO(T) > 0,$$

which is a contradiction. Now

$$\mathcal{H}(T') - \mathcal{H}(T) = \frac{2}{deg_T(u_1)+3} - \frac{2}{deg_T(u_1)+2} + \frac{2}{3+deg_T(v_1)} - \frac{2}{2+deg_T(v_1)} + \frac{2}{3+1} - \frac{2}{2+2}.$$

From Lemma 2.1 (ii), we get

$$\mathcal{H}(T') - \mathcal{H}(T) < 0,$$

which implies a contradiction. Hence, uv is not in $E(T)$ with $deg_T(u) = 2 = deg_T(v)$.

Case 2: When $uv \notin E(T)$.

Let $Nb_G(u) = \{u_1, u_2\}$ and $Nb_G(v) = \{v_1, v_2\}$. According to Case 1, the degrees of u_1, u_2, v_1 and v_2 cannot be equal to 2. WLOG, assume that u_1 and v_1 lie on the u, v-path (where u_1 and v_1 may coincide). Construct a tree $T'' \in \mathcal{CT}_{n,k}$ as follows: $T'' = T - uu_2 + vu_2$. Clearly, $deg_{T''}(u) = 1$, $deg_{T''}(v) = 3$ and $deg_{T''}(w) = deg_T(w)$ for all $w \in V(T)\backslash\{u, v\}$. Then

$$\begin{aligned} SO(T') - SO(T) &= \sqrt{deg_T^2(u_2) + 3^2} + \sqrt{deg_T^2(v_1) + 3^2} + \sqrt{deg_T^2(v_2) + 3^2} \\ &\quad + \sqrt{1^2 + deg_T^2(u_1)} - \sqrt{deg_T^2(u_2) + 2^2} - \sqrt{deg_T^2(v_1) + 2^2} \\ &\quad - \sqrt{deg_T^2(v_2) + 2^2} - \sqrt{2^2 + deg_T^2(u_1)}. \end{aligned}$$

From Lemma 2.1 (i), we achieve

$$\begin{aligned} SO(T') - SO(T) &> \sqrt{deg_T^2(v_2) + 3^2} - \sqrt{deg_T^2(v_2) + 2^2} \\ &\quad + \sqrt{1^2 + deg_T^2(u_1)} - \sqrt{2^2 + deg_T^2(u_1)}. \end{aligned}$$

From Lemma 2.1 (iii) and (iv), we have $h(d_T(u_1)) \geq h(3)$ and $g(d_T(v_1)) \geq g(4)$, respectively.

$$SO(T') - SO(T) > \sqrt{25} - \sqrt{20} + \sqrt{10} - \sqrt{13} \approx 0.084 > 0,$$

which is a contradiction. Now

$$\begin{aligned} \mathcal{H}(T'') - \mathcal{H}(T) &= \frac{2}{deg_T(u_2)+3} - \frac{2}{deg_T(u_2)+2} + \frac{2}{deg_T(v_1)+3} - \frac{2}{deg_T(v_1)+2} \\ &\quad + \frac{2}{deg_T(v_2)+3} - \frac{2}{deg_T(v_2)+2} + \frac{2}{1+deg_T(u_1)} - \frac{2}{2+deg_T(u_1)}. \end{aligned}$$

From Lemma 2.1 (vi), we have $\Psi(deg_T(u_2)) \leq \Psi(4)$, $\Psi(deg_T(v_1)) \leq \Psi(4)$, $\Psi(deg_T(v_2)) \leq \Psi(4)$ and from Lemma 2.1 (v), we have $\Phi(deg_T(u_1)) \leq \Phi(3)$. Then

$$\mathcal{H}(T'') - \mathcal{H}(T) \leq \frac{2}{7} - \frac{2}{6} + \frac{2}{7} - \frac{2}{6} + \frac{2}{7} - \frac{2}{6} + \frac{2}{4} - \frac{2}{5} \approx -0.0043 < 0,$$

which leads to a contradiction. This concludes the proof.

Lemma 2.4: *If $T \in \mathcal{CT}_{n,k}$ maximizes the Sombor index (minimizes the harmonic index), where $n-k$ is even, then (i) $n_2(T) = 0$, (ii) $n_1(T) = \frac{n}{2} + \frac{k}{2} + 1$, and (iii) $n_3(T) = \frac{n}{2} - \frac{3k}{2} - 1$.*

Proof: On the contrary, assume that $n_2(T) \neq 0$. By Lemma 2.3, we have $n_2(T) \leq 1$, which implies $n_2(T) = 1$. Since $n-k$ is even, we have $n-k = 2t_1$ for $t_1 \geq 1$. By (1.5), we get $n_1(T) + n_3(T) = 2t_1 - 1$. By Corollary 2.2, $n_1(T) + n_3(T)$ must be even. But $n_1(T) + n_3(T) = 2t_1 - 1$ is odd, which is a contradiction. Therefore, $n_2(T) = 0$.

(ii). From (1.5), (1.6) and $n_2(T) = 0$, we get

$$\begin{aligned} n &= n_1(T) + n_3(T) + k, \\ n_1(T) + 3n_3(T) &= 2n - 2 - 4k. \end{aligned} \tag{2.1}$$

The solution of the system (2.1) is $n_1(T) = \frac{n}{2} + \frac{k}{2} + 1$ and $n_3(T) = \frac{n}{2} - \frac{3k}{2} - 1$. This finishes the proof.

Lemma 2.5: *If $T \in \mathcal{CT}_{n,k}$ maximizes the Sombor index (minimizes the harmonic index), where $n-k$ is odd, then (i) $n_2(T) = 1$, (ii) $n_1(T) = \frac{n+k+1}{2}$, and (iii) $n_3(T) = \frac{n-3k-3}{2}$.*

Proof: (i). On the contrary, assume that $n_2(T) \neq 1$. By Lemma 2.3, $n_2(T) \leq 1$ which implies that $n_2(T) = 0$. Since $n-k$ is odd, we have $n-k = 2t_1 + 1$ for some $t_1 \geq 1$. Now the remaining proof is similar to Lemma 2.4.

Lemma 2.6: *If $T \in \mathcal{C}_1\mathcal{T}_{n,k}$ maximizes the Sombor index (minimizes the harmonic index), where $n-k$ is even, then (i) $m_{44}(T) \neq 0$ when $k \geq 2$, (ii) $m_{22}(T) = m_{12}(T) = m_{23}(T) = m_{24}(T) = 0$, (iii) $m_{13}(T) = 0$, (iv) $m_{33}(T) = 0$, and (v) $m_{34}(T) = \frac{3n}{2} - \frac{9k}{2} - 3$, $m_{14}(T) = \frac{n}{2} + \frac{k}{2} + 1$, and $m_{44}(T) = 4k - n + 1$.*

Proof: (i). On the contrary, assume that $m_{44}(T) = 0$ when $k \geq 2$. Then (1.4) becomes

$$m_{34}(T) = 4k - m_{14}(T) - m_{24}(T). \tag{2.2}$$

From (1.1), we deduce $m_{14}(T) \leq n_1(T)$. Then by using Lemma 2.4 (i)–(iii) and the fact that $T \in \mathcal{C}_1\mathcal{T}_{n,k}$ (for $n \leq 4k$), (2.2) becomes as

$$m_{34}(T) \geq \frac{3k-2}{2}. \tag{2.3}$$

From (1.3), we deduce

$$m_{34}(T) \leq 3n_3(T). \tag{2.4}$$

By using Lemma 2.4 (iii), and the fact that $T \in \mathcal{C}_1\mathcal{T}_{n,k}$ (for $n \leq 4k$), (2.4) becomes as

$$m_{34}(T) \leq \frac{3k-6}{2},$$

which contradicts (2.3). Hence, $m_{44}(T) \neq 0$.

(ii). This is an immediate result of Lemma 2.4 (i).

(iii). On the contrary, assume that there exists uv with $deg_T(u) = 1$ and $deg_T(v) = 3$ in T. Let $Nb_T(v)\backslash\{u\} = \{v_1, v_2\}$. Since $T \in \mathcal{C}_1\mathcal{T}_{n,k}$ and $k \geq 2$, by Lemma 2.6 (i), there exists $xy \in E(T)$ with $deg_T(x) = deg_T(y) = 4$. WLOG, let vv_1 lie on the v, x-path (where v and x may coincide). Clearly, $deg_T(v_1) \geq 3$ ($n_2(T) = 0$, by Lemma 2.4). Construct a tree $T' \in \mathcal{C}_1\mathcal{T}_{n,k}$ as follows: $T' = T - uv - vv_1 - xy + uv_1 + xv + vy$. Clearly, $deg_{T'}(w) = deg_T(w)$ for all $w \in V(T)$. Now, we discuss two cases:

Case 1: When $vx \notin E(T')$. Then

$$\begin{aligned} SO(T') - SO(T) &= \sqrt{deg_T^2(x) + deg_T^2(v)} + \sqrt{deg_T^2(v) + deg_T^2(y)} \\ &\quad + \sqrt{deg_T^2(u) + deg_T^2(v_1)} - \sqrt{deg_T^2(u) + deg_T^2(v)} \\ &\quad - \sqrt{deg_T^2(x) + deg_T^2(y)} - \sqrt{deg_T^2(v) + deg_T^2(v_1)} \\ &= \sqrt{25} + \sqrt{25} - \sqrt{10} - \sqrt{32} + \sqrt{1 + deg_T^2(v_1)} \\ &\quad - \sqrt{3^2 + deg_T^2(v_1)}. \end{aligned}$$

From Lemma 2.1 (iii), we have $h(deg_T(v_1)) \geq h(3)$. Then

$$SO(T') - SO(T) \geq \sqrt{25} + \sqrt{25} - \sqrt{10} - \sqrt{32} + \sqrt{10} - \sqrt{18} \approx 0.1 > 0,$$

which is a contradiction. Now

$$\begin{aligned} \mathcal{H}(T') - \mathcal{H}(T) &= \frac{2}{deg_T(x)+deg_T(v)} + \frac{2}{deg_T(v)+deg_T(y)} + \frac{2}{deg_T(u)+deg_T(v_1)} \\ &\quad - \frac{2}{deg_T(u)+deg_T(v)} - \frac{2}{deg_T(x)+deg_T(y)} - \frac{2}{deg_T(v)+deg_T(v_1)} \\ &= \frac{2}{4+3} + \frac{2}{3+4} - \frac{2}{1+3} - \frac{2}{4+4} + \frac{2}{1+deg_T(v_1)} - \frac{2}{3+deg_T(v_1)}. \end{aligned}$$

From Lemma 2.1 (v), we have $\Phi(deg_T(v_1)) < \Phi(3)$. Then

$$\mathcal{H}(T') - \mathcal{H}(T) \leq \frac{2}{4+3} + \frac{2}{3+4} - \frac{2}{1+3} - \frac{2}{4+4} + \frac{2}{1+3} - \frac{2}{3+3} \approx -0.011 < 0,$$

which is a contradiction.

Case 2: When $vx \in E(T')$.Then

$$SO(T') - SO(T) = \sqrt{25} + \sqrt{25} - \sqrt{10} - \sqrt{32} + \sqrt{1+16} - \sqrt{9+9} \approx 1.01 > 0.$$

which is a contradiction. Now

$$\mathcal{H}(T') - \mathcal{H}(T) = \frac{2}{4+3} + \frac{2}{3+4} - \frac{2}{1+3} - \frac{2}{4+4} + \frac{2}{1+4} - \frac{2}{3+4} \approx -0.064 < 0.$$

which is a contradiction. Therefore, $m_{13}(T) = 0$.

(iv). On the contrary, assume that there exists $uv \in E(T)$ with $deg_T(u) = 3 = deg_T(v)$. Let $Nb_T(v)\backslash\{u\} = \{v_1, v_2\}$. By Lemma 2.6 (i), there exists $e' = xy \in E(T)$ with $deg_T(x) = deg_T(y) = 4$. Now the construction of a tree $T' \in \mathcal{C}_1\mathcal{T}_{n,k}$ and calculations are the same as in the proof of Lemma 2.6 (iii). Thus, we have

$$SO(T') - SO(T) \geq \sqrt{25} + \sqrt{25} - \sqrt{10} - \sqrt{32} + \sqrt{10} - \sqrt{18} \approx 0.1 > 0,$$

and

$$\mathcal{H}(T') - \mathcal{H}(T) \leq \frac{2}{4+3} + \frac{2}{3+4} + \frac{2}{3+deg_T(v_1)} - \frac{2}{3+3} - \frac{2}{4+4} - \frac{2}{3+deg_T(v_1)} \approx -0.011 < 0,$$

which is a contradiction. Hence, $m_{33}(T) = 0$.

(v). By utilizing both Lemmas 2.4 and 2.6 (i) – (iv) in (1.1) – (1.4), we derive $m_{34}(T) = \frac{3n}{2} - \frac{9k}{2} - 3$, $m_{14}(T) = \frac{n}{2} + \frac{k}{2} + 1$, and $m_{44}(T) = 4k - n + 1$. This finishes the proof.

Lemma 2.7: If $T \in \mathcal{C}_1\mathcal{T}_{n,k}$ maximizes the Sombor index (minimizes the harmonic index), where $n - k$ is odd, then (i) $m_{44}(T) \neq 0$ when $k \geq 2$, (ii) $m_{22}(T) = 0$, (iii) $m_{12}(T) = 0$, (iv) $m_{23}(T) = 0$, (v) $m_{13}(T) = 0$, (vi) $m_{33}(T) = 0$, and (vii) $m_{34}(T) = \frac{3n-9k-9}{2}$, $m_{14}(T) = \frac{n+k+1}{2}$, $m_{24}(T) = 2$, and $m_{44}(T) = 4k - n + 1$.

Proof: (i) The proof is analogous to Lemma 2.6 (i), by utilizing Lemma 2.5 (i)–(ii).

(ii) This result directly follows from Lemma 2.5 (i).

(iii) On the contrary, assume that there exists $uv \in E(T)$ with $deg_T(u) = 1$ and $deg_T(v) = 2$. Let $Nb_T(v)\backslash\{u\} = \{v_1\}$. Clearly, $deg_T(v_1) \geq 3$ (since $n_2(T) = 1$, by Lemma 2.5). Since $T \in \mathcal{C}_1\mathcal{T}_{n,k}$ and $k \geq 2$, by Lemma 2.7 (i), it is evident that there exists $e' = xy \in E(T)$ with $deg_T(x) = deg_T(y) = 4$. Construct a tree $T' \in \mathcal{C}_1\mathcal{T}_{n,k}$ as follows: $T' = T - uv - vv_1 - xy + uv_1 + xv + vy$. Clearly, $deg_{T'}(w) = deg_T(w)$ for all $w \in V(T)$. Then

$$SO(T') - SO(T) = \sqrt{20} + \sqrt{20} - \sqrt{5} - \sqrt{32} + \sqrt{1 + deg_T^2(v_1)} - \sqrt{2^2 + deg_T^2(v_1)}.$$

From Lemma 2.1 (iii), we have $h(deg_T(v_1)) \geq h(3)$. Thus

$$SO(T') - SO(T) \geq \sqrt{25} + \sqrt{25} - \sqrt{10} - \sqrt{32} + \sqrt{10} - \sqrt{13} \approx 0.6 > 0,$$

which is a contradiction. Now

$$\mathcal{H}(T') - \mathcal{H}(T) = \frac{2}{6} + \frac{2}{6} - \frac{2}{3} - \frac{2}{8} + \frac{2}{1+deg_T(v_1)} - \frac{2}{2+deg_T(v_1)}.$$

From Lemma 2.1 (v), we have $\Phi(deg_T(v_1)) \leq \Phi(3)$. Thus

$$\mathcal{H}(T') - \mathcal{H}(T) \leq \frac{2}{3} - \frac{2}{3} - \frac{1}{4} + \frac{2}{4} - \frac{2}{5} \approx -0.15 < 0,$$

which is a contradiction. Hence, $m_{12}(T) = 0$.

(iv) On the contrary, assume that there exists $uv \in E(T)$ with $deg_T(u) = 3$ and $deg_T(v) = 2$. Let $Nb_T(v)\backslash\{u\} = \{v_1\}$. Since $T \in \mathcal{C}_1\mathcal{T}_{n,k}$ and $k \geq 2$, by Lemma 2.7 (i), there exists $e' = xy \in E(T)$ such that $deg_T(x) = deg_T(y) = 4$. Construct a tree $T' \in \mathcal{C}_1\mathcal{T}_{n,k}$ as follows: $T' = T - uv - vv_1 - xy + uv_1 + xv + vy$. Clearly, $deg_{T'}(w) = deg_T(w)$ for all $w \in V(T)$. Then

$$SO(T^*) - SO(T) = \sqrt{4^2+2^2} + \sqrt{2^2+4^2} + \sqrt{3^2+deg_T^2(v_1)} - \sqrt{3^2+2^2} - \sqrt{4^2+4^2} - \sqrt{2^2+deg_T^2(v_1)}.$$

From Lemma 2.1 (iv), we have $g(deg_T(v_1)) \geq g(4)$. Thus

$$SO(T^*) - SO(T) \geq \sqrt{20} + \sqrt{20} + \sqrt{25} - \sqrt{13} - \sqrt{32} - \sqrt{20} \approx 0.20 > 0,$$

which is a contradiction. Now

$$\mathcal{H}(T') - \mathcal{H}(T) = \frac{2}{6} + \frac{2}{6} - \frac{2}{6} - \frac{2}{8} + \frac{2}{3+deg_T(v_1)} - \frac{2}{2+deg_T(v_1)}.$$

From Lemma 2.1 (vi), we have $\Psi(deg_T(v_1)) \leq \Psi(4)$. Thus

$$\mathcal{H}(T') - \mathcal{H}(T) \leq \frac{1}{3} + \frac{1}{3} - \frac{1}{3} - \frac{1}{4} + \frac{2}{7} - \frac{2}{6} \approx -0.03 < 0.$$

which is a contradiction. Hence, $m_{23}(T) = 0$.

(v) The proof of this case is analogous to Lemma 2.6 (iii).

(vi) This proof is similar to Lemma 2.6 (iv).

(vii) By utilizing both Lemmas 2.5 and 2.7 (i) – (vi) in (1.1) – (1.4), we derive $m_{34}(T) = \frac{3n-9k-9}{2}$, $m_{14}(T) = \frac{n+k+1}{2}$, $m_{24}(T) = 2$ and $m_{44}(T) = 4k - n + 1$. This completes the result.

Lemma 2.8: *If $T \in \mathcal{C}_2\mathcal{T}_{n,k}$ maximizes the Sombor index (minimizes the harmonic index), where $n-k$ is even, then (i) $m_{22}(T) = m_{12}(T) = m_{23}(T) = m_{24}(T) = 0$, (ii) $m_{44}(T) = 0$, (iii) $m_{13}(T) = 0$, and (iv) $m_{34}(T) = \frac{7k}{2} - \frac{n}{2} - 1$, $m_{14}(T) = \frac{n}{2} + \frac{k}{2} + 1$, and $m_{33}(T) = n - 4k - 1$.*

Proof: (i). This result directly follows from Lemma 2.4 (i).

(ii). On the contrary, assume that $m_{44}(T) \neq 0$. We claim that $m_{13}(T)$ and $m_{33}(T)$ are not simultaneously 0. To prove this, assume to the contrary that $m_{13}(T) = m_{33}(T) = 0$. By using Lemma 2.8 (i) in (1.1) – (1.4), we derive $m_{14}(T) = n_1(T)$, $m_{34}(T) = 3n_3(T)$ and $m_{44}(T) = 4k - n_1(T) - 3n_3(T)$. By using Lemma 2.4, we obtain $m_{44}(T) = 8k + 2 - 2n$. Since $T \in \mathcal{C}_2\mathcal{T}_{n,k}$ (for $n \geq 4k+1$), it implies that $m_{44}(T) \leq 8k + 2 - 2(4k+1) = 0$, which is a contradiction. Hence, $m_{13}(T)$ and $m_{33}(T)$ are not simultaneously 0. Therefore, we discuss the problem in two cases.

Case 1: When $m_{13}(T) \neq 0$.

The proof is analogous to Lemma 2.6 (iii). Hence, we conclude that $m_{44}(T) = 0$.

Case 2: When $m_{33}(T) \neq 0$.

The proof is analogous to Lemma 2.6 (iv). Hence, we can conclude that $m_{44}(T) = 0$.

(iii). On the contrary, assume that $m_{13}(T) \neq 0$. Then there exists $e = xy \in E(T)$ with $deg_T(x) = 1$, $deg_T(y) = 3$, and let $Nb_T(y) \backslash \{x\} = \{y_1, y_2\}$. From (1.1), we deduce $m_{13}(T) + m_{14}(T) \leq n_1(T)$. Since $m_{13}(T) \neq 0$, it implies that $m_{14}(T) < n_1(T)$. By using Lemma 2.4 (ii) (namely, $n_1(T) = \frac{n}{2} + \frac{k}{2} + 1$), we obtain $m_{14}(T) < \frac{n}{2} + \frac{k}{2} + 1$. Since $T \in \mathcal{C}_2\mathcal{T}_{n,k}$ (for $n < 5k - 2$ and $k \geq 4$), we have $m_{14}(T) < \frac{5k-2}{2} + \frac{k}{2} + 1 = 3k$. This implies that there exists a vertex u with degree $deg_T(u) = 4$ with at most 2 pendant vertices. Let u be a furthest vertex from y, and u_1 and u_2 be the non-pendant neighbors of u. WLOG, suppose that yy_1 and u_1u are located on the y,u-path (where y and u may coincide with y_1 and u_1, respectively, and y_1 may coincide with u_1). By Lemma 2.4 (i) (that is, $n_2(T) = 0$) and Lemma 2.8 (ii) (that is, $m_{44}(T) = 0$), clear that $deg_T(u_2) \neq 2$ and $deg_T(u_2) \neq 4$. Hence, $deg_T(u_2) = 3$. Let w and z be the neighbors of u_2 other than u. Construct a tree $T' \in \mathcal{C}_2\mathcal{T}_{n,k}$ as follows: $T' = T - u_2w - u_2z + xw + zx$. Clearly, $deg_{T'}(u_2) = 1$, $deg_{T'}(x) = 3$ and $deg_{T'}(t) = deg_T(t)$ for all $t \in V(T) \backslash \{u_2, x\}$. Then

$$\begin{aligned} SO(T') - SO(T) &= \sqrt{deg_T^2(w) + 3^2} + \sqrt{deg_T^2(z) + 3^2} + \sqrt{3^2 + 3^2} \\ &\quad - \sqrt{4^2 + 1} + \sqrt{4^2 + 3^2} - \sqrt{3^2 + deg_T^2(w)} \\ &\quad - \sqrt{3^2 + deg_T^2(z)} - \sqrt{3^2 + 1} \approx 0.2 > 0. \end{aligned}$$

which is a contradiction. Now

$$\begin{aligned} \mathcal{H}(T') - \mathcal{H}(T) &= \frac{2}{deg_T(w)+3} + \frac{2}{deg_T(z)+3} + \frac{2}{3+3} + \frac{2}{4+1} - \frac{2}{4+3} \\ &\quad - \frac{2}{3+deg_T(w)} - \frac{2}{3+deg_T(z)} - \frac{2}{1+3} \approx -0.05 < 0. \end{aligned}$$

which is a contradiction. Hence, $m_{13}(T) = 0$.

(iv). By utilizing both Lemmas 2.4 and 2.8 (i) – (iv) in (1.1) – (1.4), we derive $m_{34}(T) = \frac{7k}{2} - \frac{n}{2} - 1$, $m_{14}(T) = \frac{n}{2} + \frac{k}{2} + 1$, and $m_{33}(T) = n - 4k - 1$. This finishes the proof.

Lemma 2.9: If $T \in \mathcal{C}_2\mathcal{T}_{n,k}$ maximizes the Sombor index (minimizes the harmonic index), where $n - k$ is odd, then (i) $m_{22}(T) = 0$, (ii) $m_{12}(T) = 0$, (iii) $m_{44}(T) = 0$, (iv) $m_{13}(T) = 0$, (v) $m_{24}(T) = 2$ and $m_{23}(T) = 0$, and (vi) $m_{34}(T) = \frac{7k-n-5}{2}$, $m_{14}(T) = \frac{n+k+1}{2}$, and $m_{33}(T) = n - 4k - 1$.

Proof: (i). This result directly follows from Lemma 2.5 (i).

(ii). On the contrary, assume that $m_{12}(T) \neq 0$. Then there exists $xy \in E(T)$ with $deg_T(x) = 1$ and $deg_T(y) = 2$. Let y_1 be the neighbor of y

distinct from x, and let u be a furthest vertex from y with degree 4, where $Nb_T(u) = \{u_i \mid 1 \leq i \leq 4\}$. WLOG, assume that yy_1 and uu_4 exist on the u, y-path, and y_1 and u_4 may coincide. From Lemma 2.5 (i) (that is, $n_2(T) = 1$), it is clear that $3 \leq deg_T(u_4) \leq 4$. Construct a tree $T' \in \mathcal{C}_2\mathcal{T}_{n,k}$ as follows: $T' = T - \{uu_i \mid 1 \leq i \leq 3\} + \{xu_i \mid 1 \leq i \leq 3\}$. Clearly, $deg_{T'}(u) = 1$, $deg_{T'}(x) = 4$ and $deg_{T'}(w) = deg_T(w)$ for all $w \in V(T) \backslash \{u, x\}$. Then

$$\begin{aligned} SO(T') - SO(T) &= \sum_{i=1}^{3} \left(\sqrt{deg_T^2(u_i) + 4^2} - \sqrt{4^2 + deg_T^2(u_i)}\right) \\ &\quad + \sqrt{4^2 + 2^2} - \sqrt{1^2 + 2^2} + \sqrt{deg_T^2(u_4) + 1^2} \\ &\quad - \sqrt{4^2 + deg_T^2(u_4)}. \end{aligned}$$

From Lemma 2.1 (iii), we have $h(deg_T(u_4)) \geq h(3)$. Thus

$$SO(T') - SO(T) \geq \sqrt{4^2 + 2^2} + \sqrt{3^2 + 1^2} - \sqrt{4^2 + 3^2} - \sqrt{1^2 + 2^2} \approx 0.398 > 0,$$

which is a contradiction. Now

$$\begin{aligned} \mathcal{H}(T') - \mathcal{H}(T) &= \sum_{i=1}^{3} \left(\frac{2}{deg_T(u_i)+4} - \frac{2}{deg_T(u_i)+4}\right) + \frac{2}{4+2} - \frac{2}{1+2} \\ &\quad + \frac{2}{deg_T(u_4)+1} - \frac{2}{4+deg_T(u_4)}. \end{aligned}$$

From Lemma 2.1 (v), we have $\Phi(deg_T(v_4)) \leq \Phi(3)$. Thus

$$\mathcal{H}(T') - \mathcal{H}(T) \leq \frac{2}{4+2} - \frac{2}{1+2} + \frac{2}{3+1} - \frac{2}{4+3} \approx -0.11 < 0,$$

which is a contradiction. Hence, $m_{12}(T) = 0$.

(iii). On the contrary, assume that $m_{44}(T) \neq 0$. Then there exists $xy \in E(T)$ with $deg_T(x) = deg_T(y) = 4$. We claim that $m_{13}(T)$, $m_{23}(T)$ and $m_{33}(T)$ are not simultaneously 0. To prove this, assume that $m_{13}(T) = m_{23}(T) = m_{33}(T) = 0$. By utilizing Lemmas 2.9 (i)–(ii) in (1.1) – (1.4), we derive $m_{14}(T) = n_1(T)$, $m_{24}(T) = 2n_2(T)$, $m_{34}(T) = 3n_3(T)$ and $m_{44}(T) = 4k - n_1(T) - 3n_3(T) - 2n_2(T)$. By using Lemma 2.5, we have $m_{44}(T) = 8k + 2 - 2n$. Since $T \in \mathcal{C}_2\mathcal{T}_{n,k}$ (for $n \geq 4k + 1$), it implies that $m_{44}(T) \leq 8k + 2 - 2(4k + 1) = 0$, which is a contradiction. Hence, $m_{13}(T)$, $m_{23}(T)$ and $m_{33}(T)$ are not simultaneously 0. Therefore, we distinguish the following cases.

Case 1: When $m_{13}(T) \neq 0$.

The proof is analogous to Lemma 2.6 (iii). Hence, we conclude that $m_{44}(T) = 0$.

Case 2: When $m_{33}(T) \neq 0$.

The proof is analogous to Lemma 2.6 (iv). Hence, we can conclude that $m_{44}(T) = 0$.

Case 3: When $m_{23}(T) \neq 0$.

The proof is analogous to Lemma 2.7 (iv). Hence, we can conclude that $m_{44}(T) = 0$.

From each case, we obtain $m_{44}(T) = 0$.

(iv). This proof is analogous to that of Lemma 2.8 (iii) up to the y, u-path, employing the Lemma 2.5 (ii). Since u_2 is the non-pendant neighbor of 4 degree vertex u, by Lemma 2.9 (iii) (that is, $m_{44}(T) = 0$), it implies that $deg_T(u_2) \neq 4$. Therefore, $deg_T(u_2) \in \{2,3\}$. Now we discuss the problem in the following cases.

Case 1: When $deg_T(u_2) = 3$.

The proof is analogous to Lemma 2.8 (iii).

Case 2: When $deg_T(u_2) = 2$.

Let w be the neighbor of u_2 other than u. Construct a tree $T' \in \mathcal{C}_2\mathcal{T}_{n,k}$ as follows: $T' = T - u_2w + xw$. Clearly, $deg_{T'}(u_2) = 1$, $deg_{T'}(x) = 2$ and $deg_{T'}(t) = deg_T(t)$ for all $w \in V(T)\backslash\{u_2, x\}$. Now

$$SO(T') - SO(T) = \sqrt{deg_T^2(w) + 2^2} + \sqrt{2^2 + 3^2} + \sqrt{4^2 + 1} - \sqrt{4^2 + 2^2}$$
$$-\sqrt{deg_T^2(w) + 2^2} - \sqrt{1 + 3^2} \approx 0.09 > 0,$$

which is a contradiction. Then

$$\mathcal{H}(T') - \mathcal{H}(T) = \frac{2}{deg_T(w)+2} + \frac{2}{2+3} + \frac{2}{4+1} - \frac{2}{4+2} - \frac{2}{2+deg_T(w)} - \frac{2}{1+3} \approx -0.03 < 0,$$

which is a contradiction. Hence, $m_{13}(T) = 0$.

(v). On the contrary, assume that $m_{24}(T) \neq 2$. By Lemma 2.5 (i), clear that $m_{24}(T)2$. Now, it is evident that $m_{24}(T) < 2$. Let u be the vertex of degree 2 and $Nb_T(u) = \{u_1, u_2\}$. WLOG, assume that $deg_T(u_2) = 3$ and $deg_T(u_1) \in \{3,4\}$ (by Lemma 2.9 (i)–(ii)). Next, we distinguish the following cases.

Case 1: When $deg_T(u_1) = deg_T(u_2) = 3$.

Let x be a vertex of degree 4 and x' be its non-pendant neighbor. By Lemmas 2.5 (i) and 2.9 (iii), it is evident that $deg_T(x') = 3$. WLOG, let u, x-path containing uu_2 and xx' (where x' and u_2 may coincide). Construct $T' \in \mathcal{C}_2\mathcal{T}_{n,k}$ as follows: $T' = T - uu_1 - uu_2 - xx' + xu + x'u + u_1u_2$. Clearly, $deg_{T'}(w) = deg_T(w)$ for all $w \in V(T)$. Then

$$\begin{aligned}SO(T') - SO(T) &= \sqrt{deg_T^2(x) + deg_T^2(u)} + \sqrt{deg_T^2(x') + deg_T^2(u)} \\ &\quad + \sqrt{deg_T^2(u_1) + deg_T^2(u_2)} - \sqrt{deg_T^2(u) + deg_T^2(u_1)} \\ &\quad - \sqrt{deg_T^2(u_2) + deg_T^2(u)} - \sqrt{deg_T^2(x) + deg_T^2(x')} \\ &= \sqrt{4^2 + 2^2} + \sqrt{3^2 + 2^2} + \sqrt{3^2 + 3^2} - \sqrt{2^2 + 3^2} \\ &\quad - \sqrt{3^2 + 2^2} - \sqrt{4^2 + 3^2} \\ &\approx 0.10 > 0,\end{aligned}$$

which is a contradiction. Now

$$\begin{aligned}\mathcal{H}(T') - \mathcal{H}(T) &= \frac{2}{deg_T(x)+deg_T(u)} + \frac{2}{deg_T(x\prime)+deg_T(u)} + \frac{2}{deg_T(u_1)+deg_T(u_2)} \\ &- \frac{2}{deg_T(u)+deg_T(u_1)} - \frac{2}{deg_T(u_2)+deg_T(u)} - \frac{2}{deg_T(x)+deg_T(x\prime)} \\ &= \frac{2}{4+2} + \frac{2}{3+2} + \frac{2}{3+3} - \frac{2}{2+3} - \frac{2}{3+2} - \frac{2}{4+3} = -0.019 < 0,\end{aligned}$$

which is a contradiction.

Case 2: When $deg_T(u_1) = 4$ and $deg_T(u_2) = 3$.

Firstly, let's discuss the neighbors of 4 degree vertices. By Lemma 2.5 (ii), we have $n_1(T) = \frac{n+k+1}{2}$. Since $T \in \mathcal{C}_2\mathcal{T}_{n,k}$ for $4k < n < 5k - 2$, we can infer that

$$2k < \frac{5k+1}{2} < n_1(T) < \frac{6k-1}{2} < 3k. \tag{2.5}$$

From Lemma 2.9 (ii) and (iv), it is evident that pendant vertices are adjacent to k vertices. Subsequently, based on (2.5), we conclude that there exists a vertex of degree 4 with exactly 3 pendant neighbors and another vertex of degree 4 with at most 2 pendant neighbors. Now, focusing on the pendant vertices, we examine the following subcases:

Subcase 1: When u_1 has three pendant neighbors.

Let y be another vertex of degree 4 with at most 2 pendant neighbors. Assume that y_1 and y_2 are the non-pendant neighbors of y. By Lemmas 2.5 (i) and 2.9 (iii), it is evident that $deg_T(y_1) = deg_T(y_2) = 3$. WLOG, we suppose that there exists a u_1, y-path containing uu_2 and yy_2 (where u_2 and y_2 may coincide). Construct a tree $T'' \in \mathcal{C}_2\mathcal{T}_{n,k}$ as follows: $T'' = T - yy_1 - yy_2 + uy + u_2y + y_1y_2$. Clearly, $deg_{T''}(w) = deg_T(w)$ for all $w \in V(T)$. Then

$$\begin{aligned}SO(T'') - SO(T) &= \sqrt{deg_T^2(y) + deg_T^2(u)} + \sqrt{deg_T^2(u_2) + deg_T^2(y)} \\ &+ \sqrt{deg_T^2(y_1) + deg_T^2(y_2)} - \sqrt{deg_T^2(y) + deg_T^2(y_1)} \\ &- \sqrt{deg_T^2(y_2) + deg_T^2(y)} - \sqrt{deg_T^2(u) + deg_T^2(u_2)} \\ &= \sqrt{4^2 + 2^2} + \sqrt{4^2 + 3^2} + \sqrt{3^2 + 3^2} - \sqrt{4^2 + 3^2} \\ &- \sqrt{4^2 + 3^2} - \sqrt{2^2 + 3^2} \\ &\approx 0.10 > 0,\end{aligned}$$

which is a contradiction. Now

$$\begin{aligned}\mathcal{H}(T'') - \mathcal{H}(T) &= \frac{2}{deg_T(y)+deg_T(u)} + \frac{2}{deg_T(u_2)+deg_T(y)} + \frac{2}{deg_T(y_1)+deg_T(y_2)} \\ &- \frac{2}{deg_T(y)+deg_T(y_1)} - \frac{2}{deg_T(y_2)+deg_T(y)} - \frac{2}{deg_T(u)+deg_T(u_2)} \\ &= \frac{2}{4+2} + \frac{2}{4+3} + \frac{2}{3+3} - \frac{2}{4+3} - \frac{2}{4+3} - \frac{2}{2+3} \approx -0.019 < 0,\end{aligned}$$

which is a contradiction.

Subcase 2: When u_1 has at most 2 pendant neighbors.

Let u'_1 be any non-pendant neighbor of u_1 other than u. Assume that v be any pendant vertex and $N_v(T) = \{x\}$. From Lemmas 2.9 (ii) and (iv), it is clear that $deg_T(x) = 4$. Then there exists a u_1, v-path that contains uu_2 and xx', where x' be any non-pendant neighbor of x (u_2 and x' may coincide). By Lemmas 2.5 (i) and 2.9 (iii), it is evident that $deg_T(x') = deg_T(u'_1) = 3$. Construct a tree $T''' \in \mathcal{C}_2\mathcal{T}_{n,k}$ as follows: $T''' = T - u'_1u_1 - uu_2 - x'x + ux + u_1x' + u'_1u_2$. Clearly, $deg_{T'''}(w) = deg_T(w)$ for all $w \in V(T)$. Then

$$\begin{aligned}
SO(T''') - SO(T) &= \sqrt{deg_T^2(x) + deg_T^2(u)} + \sqrt{deg_T^2(u_1') + deg_T^2(u_2)} \\
&\quad + \sqrt{deg_T^2(u_2) + deg_T^2(x')} - \sqrt{deg_T^2(u_1') + deg_T^2(u_1)} \\
&\quad - \sqrt{deg_T^2(u_2) + deg_T^2(u)} - \sqrt{deg_T^2(x') + deg_T^2(x)} \\
&= \sqrt{4^2 + 2^2} + \sqrt{3^2 + 3^2} + \sqrt{3^2 + 4^2} - \sqrt{3^2 + 4^2} \\
&\quad - \sqrt{2^2 + 3^2} - \sqrt{4^2 + 3^2} \\
&\approx 0.10 > 0,
\end{aligned}$$

which is a contradiction. Now

$$\begin{aligned}
\mathcal{H}(T''') - \mathcal{H}(T) &= \frac{2}{\sqrt{deg_T(x) + deg_T(u)}} + \frac{2}{\sqrt{deg_T(u_1') + deg_T(u_2)}} \\
&\quad + \frac{2}{\sqrt{deg_T(u_1) + deg_T(x')}} - \frac{2}{\sqrt{deg_T(u_1') + deg_T(u_1)}} \\
&\quad - \frac{2}{\sqrt{deg_T(u_2) + deg_T(u)}} - \frac{2}{\sqrt{deg_T(x') + deg_T(x)}} \\
&= \frac{2}{4+2} + \frac{2}{3+3} + \frac{2}{3+4} - \frac{2}{3+4} - \frac{2}{2+3} - \frac{2}{4+3} \\
&\approx -0.019 > 0,
\end{aligned}$$

which is a contradiction. In each case, we get a contradiction. Therefore, $m_{24}(T) = 2$. Since $n_2(T) = 1$ and $m_{24}(T) = 2$, it implies $m_{23}(T) = 0$.

(vi) By utilizing both Lemmas 2.5 (i) – (iii) and 2.9 (i) – (v) in (1.1) – (1.4), we derive $m_{34}(T) = \frac{7k-n-5}{2}$, $m_{14}(T) = \frac{n+k+1}{2}$ and $m_{33}(T) = n - 4k - 1$. This establishes the proof.

Lemma 2.10: *If $T \in \mathcal{C}_3\mathcal{T}_{n,k}$ maximizes the Sombor index (minimizes the harmonic index), where $n - k$ is even, then (i) $m_{12}(T) = m_{22}(T) = m_{23}(T) = m_{24}(T) = 0$, (ii) $m_{44}(T) = 0$, (iii) $m_{14}(T) = 3k$, and (iv) $m_{34}(T) = k$, $m_{13}(T) = \frac{n}{2} - \frac{5k}{2} + 1$, and $m_{33}(T) = \frac{n}{2} - \frac{3k}{2} - 2$.*

Proof: (i). This result directly follows from Lemma 2.4 (i).

(ii). The proof of this case is similar to Lemma 2.8 (ii).

(iii). On the contrary, assume that $m_{14}(T) \neq 3k$. Then we have $m_{14}(T) > 3k$ or $m_{14}(T) < 3k$. If $m_{14}(T) > 3k$, then there exists a vertex of degree 4 with 4 pendant neighbors, which is not possible. Therefore, we consider the case when $m_{14}(T) < 3k$. We further claim that if $m_{14}(T) < 3k$, then $m_{13}(T) > 0$. On the contrary, assume that $m_{13}(T) = 0$. From Lemma 2.10 (i), (1.1), and $m_{13}(T) = 0$, we have $m_{14}(T) = n_1(T)$. This implies $n_1(T) < 3k$. By using Lemma 2.4 (ii), we deduce $\frac{n}{2} + \frac{k}{2} + 1 < 3k$. Consequently, $n < 5k - 2$ which leads to a contradiction, as $T \in \mathcal{C}_3\mathcal{T}_{n,k}$. Hence, $m_{13}(T) > 0$.

Then there exists $xy \in E(T)$ with $deg_T(x) = 1$ and $deg_T(y) = 3$. Moreover, $m_{14}(T) < 3k$ implies that there exists a vertex u with degree $deg_T(u) = 4$ with at most 2 pendant vertices. Let u_1 and u_2 be the non-pendant neighbors of u. Let y_1 and y_2 be the neighbors of y other than x. WLOG, let yy_1 and u_1u be located on the y,u-path (where y_1 and u_1 may coincide). By Lemmas 2.10 (ii) and 2.4 (i), it is clear that $deg_T(u_2) = 3$. Let w and z be the neighbors of u_2 other than u. Construct a tree $T' \in \mathcal{C}_3\mathcal{T}_{n,k}$ as follows: $T' = T - u_2w - u_2z + xw + zx$. Clearly, $deg_{T'}(u_2) = 1$, $deg_{T'}(x) = 3$ and $deg_{T'}(w) = deg_T(w)$ for all $w \in V(T)\backslash\{u_2, x\}$. Now

$$\begin{aligned} SO(T') - SO(T) &= \sqrt{deg_T^2(w) + 3^2} + \sqrt{deg_T^2(z) + 3^2} + \sqrt{3^2 + 3^2} \\ &\quad + \sqrt{4^2 + 1^2} - \sqrt{4^2 + 3^2} - \sqrt{3^2 + deg_T^2(w)} \\ &\quad - \sqrt{3^2 + deg_T^2(z)} - \sqrt{1^2 + 3^2} \approx 0.20 > 0. \end{aligned}$$

This is a contradiction. Then

$$\begin{aligned} \mathcal{H}(T') - \mathcal{H}(T) &= \frac{2}{deg_T(w)+3} + \frac{2}{deg_T(z)+3} + \frac{2}{3+3} + \frac{2}{4+1} - \frac{2}{4+3} \\ &\quad - \frac{2}{3+deg_T(w)} - \frac{2}{3+deg_T(z)} - \frac{2}{1+3} \approx -0.05 < 0. \end{aligned}$$

This leads a contradiction. Hence, $m_{14}(T) = 3k$.

(iv) By utilizing both Lemmas 2.4 (i) – (ii) and 2.10 (i) – (v) in (1.1) – (1.4), we derive $m_{34}(T) = k$, $m_{13}(T) = \frac{n}{2} - \frac{5k}{2} + 1$ and $m_{33}(T) = \frac{n}{2} - \frac{3k}{2} - 2$. This concludes the proof.

Lemma 2.11: *If $T \in \mathcal{C}_3\mathcal{T}_{n,k}$ maximizes the Sombor index (minimizes the harmonic index), where $n - k$ is odd, then (i) $m_{22}(T) = 0$, (ii) $m_{12}(T) = 0$, (iii) $m_{44}(T) = 0$, (iv) $m_{23}(T) = 1$, (v) $m_{14}(T) = 3k$, and (vi) $m_{24}(T) = 1$, $m_{13}(T) = \frac{n-5k+1}{2}$, $m_{33}(T) = \frac{n-3k-5}{2}$ and $m_{34}(T) = k - 1$.*

Proof: (i). This result directly follows from Lemma 2.5 (i).

(ii). The proof is similar to that of Lemma 2.9 (ii).

(iii). This proof is analogous to Lemma 2.9 (iii).

(iv). On the contrary, assume that $m_{23}(T) \neq 1$. Let u be the vertex with degree 2 and let u_1 and u_2 be its neighbors. From Lemma 2.5 (i), it is clear that $m_{23}(T) \leq 2$. Therefore, $m_{23}(T) = 0$ or $m_{23}(T) = 2$. Next we have the following two cases:

Case 1: When $m_{23}(T) = 2$ and $deg_T(u_1) = deg_T(u_2) = 3$. This case is analogous to Lemma 2.9 (iv).

Case 2: When $m_{23}(T) = 0$ and $deg_T(u_1) = deg_T(u_2) = 4$. We claim $m_{24}(T) = 2$, then $m_{13}(T) \neq 0$. To prove this, assume that $m_{13}(T) = 0$. From Lemma 2.11 (ii), $m_{13}(T) = 0$ and (1.1), we have $m_{14}(T) = n_1(T)$. By using Lemma 2.5 (ii), we obtain $m_{14}(T) = \frac{n+k+1}{2}$. Since $T \in \mathcal{C}_3\mathcal{T}_{n,k}$ $(n > 5k-3)$, we have $m_{14}(T) > \frac{5k-3+k+1}{2} = 3k-1$. However, it is easy to see that for $n \geq 10$ and $k \geq 2$, if $m_{24}(T) = 2$, then $m_{14}(T) < 3k$. This gives a contradiction. Assume that there exists $xy \in E(T)$ with $deg_T(x) = 3$ and $deg_T(y) = 1$. WLOG, let u_1 does not lie on the u, x-path. Construct a tree $T' \in \mathcal{C}_3\mathcal{T}_{n,k}$ as follows: $T' = T - uu_1 + yu_1$. Clearly, $deg_{T'}(u) = deg_T(u) - 1$, $deg_{T'}(y) = deg_T(y) + 1$ and $deg_{T'}(w) = deg_T(w)$ for all $w \in V(T)\backslash\{u, y\}$. Then

$$\begin{aligned} SO(T') - SO(T) &= \sqrt{(d_T(y)+1)^2 + d_T^2(u_1)} - \sqrt{deg_T^2(u) + deg_T^2(u_1)} \\ &\quad - \sqrt{deg_T^2(y) + deg_T^2(x)} + \sqrt{(deg_T(y)+1)^2 + deg_T^2(x)} \\ &\quad + \sqrt{(deg_T(u)-1)^2 + deg_T^2(u_2)} - \sqrt{deg_T^2(u) + deg_T^2(u_2)} \\ &= \sqrt{2^2+4^2} + \sqrt{1^2+4^2} + \sqrt{2^2+3^2} \\ &\quad - \sqrt{2^2+4^2} - \sqrt{2^2+4^2} - \sqrt{3^2+1^2} \\ &\approx 0.09 > 0. \end{aligned}$$

This is a contradiction. Now

$$\begin{aligned} \mathcal{H}(T') - \mathcal{H}(T) &= \frac{2}{deg_T(y)+1+deg_T(u_1)} + \frac{2}{deg_T(u)-1+deg_T(u_2)} + \frac{2}{deg_T(y)+1+deg_T(x)} \\ &\quad - \frac{2}{deg_T(u)+deg_T(u_1)} - \frac{2}{deg_T(u)+deg_T(u_2)} - \frac{2}{deg_T(y)+deg_T(x)} \\ &= \frac{2}{2+4} + \frac{2}{1+4} + \frac{2}{2+3} - \frac{2}{2+4} - \frac{2}{2+4} - \frac{2}{3+1} \approx -0.030 < 0. \end{aligned}$$

This leads to a contradiction. Hence, $m_{23}(T) = 1$.

(v). On the contrary, assume that $m_{14}(T) \neq 3k$. Then we have $m_{14}(T) > 3k$ or $m_{14}(T) < 3k$. However, $m_{14}(T) < 3k$ because otherwise it would imply the existence of a vertex of degree 4 with four pendant neighbors. We further claim that if $m_{14}(T) < 3k$, then $m_{13}(T) > 0$. On the contrary, assume that $m_{13}(T) = 0$. By Lemma 2.11 (ii) and (1.1), we have $m_{14}(T) = n_1(T)$. This implies $n_1(T) < 3k$. By using Lemma 2.5 (ii), we obtain $\frac{n+k+1}{2} < 3k$. This gives $n < 5k-1$ which is a contradiction as $T \in \mathcal{C}_3\mathcal{T}_{n,k}$. Hence, $m_{13}(T) > 0$.

Then there exists $xy \in E(T)$ with $deg_T(x) = 1$ and $deg_T(y) = 3$. Moreover, $m_{14}(T) < 3k$ implies that there exists a vertex u with $deg_T(u) = 4$ with at most 2 pendant vertices. Let u_1 and u_2 be the non-pendant neighbors of u. Let y_1 and y_2 be neighbors of y other than x. WLOG, let yy_1 and u_1u lie on the y,u-path. By Lemma 2.11 (iii), it implies that $deg_T(u_2) \neq 4$. Therefore, $deg_T(u_2) \in \{2,3\}$. Now, arises following cases:

Case 1: When $deg_T(u_2) = 3$. This case is similar to Case 1 of Lemma 2.10 (iii).

Case 2: When $deg_T(u_2) = 2$. Let w be the neighbor of u_2 other than u. Construct a tree $T' \in \mathcal{C}_3\mathcal{T}_{n,k}$ as follows: $T' = T - u_2w + xw$. Clearly, $deg_{T'}(u_2) = deg_T(u_2) - 1$, $deg_{T'}(x) = deg_T(x) + 1$ and $deg_{T'}(w) = deg_T(w)$ for all $w \in V(T)\backslash\{u_2, x\}$. Now

$$SO(T') - SO(T) = \sqrt{deg_T^2(w) + 2^2} + \sqrt{2^2 + 3^2} + \sqrt{4^2 + 1^2} - \sqrt{4^2 + 2^2}$$
$$- \sqrt{deg_T^2(w) + 2^2} - \sqrt{1^2 + 3^2} \approx 0.09 > 0.$$

This is a contradiction. Now

$$\mathcal{H}(T') - \mathcal{H}(T) = \frac{2}{deg_T(w)+2} + \frac{2}{2+3} + \frac{2}{4+1} - \frac{2}{4+2} - \frac{2}{deg_T(w)+2} - \frac{2}{1+3} \approx -0.03 < 0,$$

which is a contradiction. Hence, $m_{13}(T) = 0$.

(vi). By utilizing both Lemmas 2.11 (i) – (v) and 2.5 in (1.1) – (1.4), we derive $m_{24}(T) = 1$, $m_{13}(T) = \frac{n-5k+1}{2}$, $m_{33}(T) = \frac{n-3k-5}{2}$ and $m_{34}(T) = k - 1$. This establishes the proof.

Theorem 2.12: *Let $T \in \mathcal{CT}_{n,k}$ be a tree with maximum Sombor index (minimum harmonic index). Then the values of $SO(T)$ ($\mathcal{H}(T)$) are given in Table 1.*

Table 1

Extremal chemical trees in $\mathcal{CT}_{n,k}$ for Sombor index and harmonic index

n and k	$\mathcal{CT}_{n,k}$	Maximum value of SO index	Minimum value of $\mathcal{H}$ index
$n = 5$ and $k = 1$	$\{S_5\}$	$4\sqrt{17}$	$6/5$
$n = 6$ and $k = 1$	$\{S_{4,2}\}$	$3\sqrt{17} + \sqrt{20} + \sqrt{5}$	$7/5$
$n - k$ is even	$\mathcal{C}_1\mathcal{T}_{n,k}$	$(\frac{15+\sqrt{17}-8\sqrt{2}}{2})n + (\frac{\sqrt{17}-45+32\sqrt{2}}{2})k + \sqrt{17} + 4\sqrt{2} - 15$	$\frac{53n-12k-29}{140}$
$n - k$ is odd	$\mathcal{C}_1\mathcal{T}_{n,k}$	$(\frac{15+\sqrt{17}-8\sqrt{2}}{2})n + (\frac{\sqrt{17}-45+32\sqrt{2}}{2})k + \frac{\sqrt{17}-45}{2} + 4\sqrt{2} + 4\sqrt{5}$	$\frac{159n-39k-71}{420}$
$n - k$ is even	$\mathcal{C}_2\mathcal{T}_{n,k}$	$(\frac{6\sqrt{2}+\sqrt{17}-5}{2})n + (\frac{35+\sqrt{17}-24\sqrt{2}}{2})k + \sqrt{17} - 5 - 3\sqrt{2}$	$\frac{41n-14k-23}{105}$

$n-k$ is odd	$\mathcal{C}_2\mathcal{T}_{n,k}$	$(\frac{6\sqrt{2}+\sqrt{17}-5}{2})n+(\frac{35+\sqrt{17}-24\sqrt{2}}{2})k$ $+4\sqrt{5}-3\sqrt{2}+\frac{\sqrt{17}-25}{2}$	$\frac{41n-7k-19}{105}$
$n-k$ is even	$\mathcal{C}_3\mathcal{T}_{n,k}$	$(\frac{\sqrt{10}+3\sqrt{2}}{2})n+(5+3\sqrt{17}$ $-\frac{5\sqrt{10}+9\sqrt{2}}{2})k+\sqrt{10}-6\sqrt{2}$	$\frac{175n-111k-70}{420}$
$n-k$ is odd	$\mathcal{C}_3\mathcal{T}_{n,k}$	$(\frac{\sqrt{10}+3\sqrt{2}}{2})n+(5-\frac{5\sqrt{10}+9\sqrt{2}}{2}$ $+3\sqrt{17})k+\sqrt{13}-5+\frac{2\sqrt{20}+\sqrt{10}}{2}$	$\frac{175n-615k-22}{420}$

Proof: It is easily seen that $\mathcal{CT}_{5,1}=\{S_5\}$ and $\mathcal{CT}_{6,1}=\{S_{4,2}\}$. The results for the extremal values of S_5 and $S_{4,2}$ are given in Table 1 by direct calculation. We now discuss the problem in the following cases:

Case 1: If $T\in\mathcal{C}_1\mathcal{T}_{n,k}$ and $n-k$ is even, then by applying Lemma 2.6 in (1.7) and (1.8), respectively, we obtain

$$\mathcal{H}(T)\ =\frac{53n-12k-29}{140},$$
$$SO(T)\ =\left(\frac{15+\sqrt{17}-8\sqrt{2}}{2}\right)n+\left(\frac{\sqrt{17}-45+32\sqrt{2}}{2}\right)k+\sqrt{17}+4\sqrt{2}-15.$$

Case 2: If $T\in\mathcal{C}_1\mathcal{T}_{n,k}$ and $n-k$ is odd, then by applying Lemma 2.7 in (1.7) and (1.8), respectively, we obtain

$$\mathcal{H}(T)\ =\frac{159n-39k-71}{420},$$
$$SO(T)\ =\left(\frac{15+\sqrt{17}-8\sqrt{2}}{2}\right)n+\left(\frac{\sqrt{17}-45+32\sqrt{2}}{2}\right)k+\frac{\sqrt{17}-45}{2}+4\sqrt{2}+4\sqrt{5}.$$

Case 3: If $T\in\mathcal{C}_2\mathcal{T}_{n,k}$ and $n-k$ is even, then by applying Lemma 2.8 in (1.7) and (1.8), respectively, we obtain

$$\mathcal{H}(T)\ =\frac{41n-14k-23}{105},$$
$$SO(T)\ =\left(\frac{6\sqrt{2}+\sqrt{17}-5}{2}\right)n+\left(\frac{35+\sqrt{17}-24\sqrt{2}}{2}\right)k+\sqrt{17}-5-3\sqrt{2}.$$

Case 4: If $T\in\mathcal{C}_2\mathcal{T}_{n,k}$ and $n-k$ is odd, then by applying Lemma 2.9 in (1.7) and (1.8), respectively, we obtain

$$\mathcal{H}(T)\ =\frac{41n-7k-19}{105},$$
$$SO(T)\ =\left(\frac{6\sqrt{2}+\sqrt{17}-5}{2}\right)n+\left(\frac{35+\sqrt{17}-24\sqrt{2}}{2}\right)k+4\sqrt{5}-3\sqrt{2}+\frac{\sqrt{17}-25}{2}.$$

Case 5: If $T\in\mathcal{C}_3\mathcal{T}_{n,k}$ and $n-k$ is even, then by applying Lemma 2.10 in (1.7) and (1.8), respectively, we obtain

$$\mathcal{H}(T)\ =\frac{5}{12}n-\frac{37}{140}k-\frac{1}{6},$$
$$SO(T)\ =\left(\frac{\sqrt{10}+3\sqrt{2}}{2}\right)n+\left(5+3\sqrt{17}-\frac{5\sqrt{10}+9\sqrt{2}}{2}\right)k+\sqrt{10}-6\sqrt{2}.$$

Case 6: If $T \in \mathcal{C}_3\mathcal{T}_{n,k}$ and $n-k$ is odd, then by applying Lemma 2.11 in (1.7) and (1.8), respectively, we obtain

$$\mathcal{H}(T) = \frac{5}{12}n - \frac{41}{28}k - \frac{19}{140},$$

$$SO(T) = \left(\frac{\sqrt{10}+3\sqrt{2}}{2}\right)n + \left(5 - \frac{5\sqrt{10}+9\sqrt{2}}{2} + 3\sqrt{17}\right)k + \sqrt{13} - 5 + \frac{2\sqrt{20}+\sqrt{10}}{2}.$$

This finishes the proof.

3. Construction of extremal trees

From Theorem 2.12, we found chemical trees in the class $\mathcal{CT}_{n,k}$ that maximize the Sombor index and the same trees simultaneously minimize the harmonic index. In this section, we construct the corresponding extremal chemical trees. Notably, $\mathcal{CT}_{n,k}$ has only S_4 and $S_{4,2}$ when $n = 5$, $k = 1$ and $n = 6$, $k = 1$, respectively. Thus, let us construct the extremal chemical trees, excluding the cases where $n \in \{5,6\}$ and $k = 1$.

Corollary 3.1: If $T \in \mathcal{C}_1\mathcal{T}_{n,k}$ and $n-k$ is even, then the tree T with maximum SO index and minimum harmonic index is shown in Fig. 1.

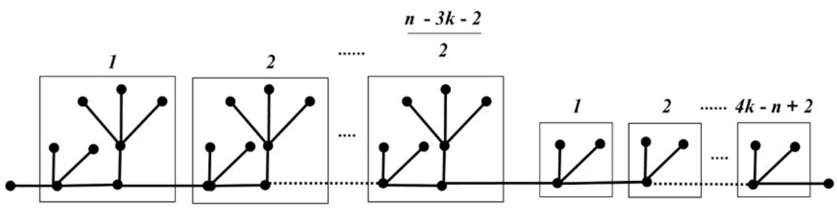


Figure 1
$\boldsymbol{T \in \mathcal{C}_1\mathcal{T}_{n,k}}$ **when** $\boldsymbol{n-k}$ **is even.**

Corollary 3.2: *If $T \in \mathcal{C}_1\mathcal{T}_{n,k}$ and $n-k$ is odd, then the tree T with maximum SO index and minimum harmonic index is shown in Fig. 2.*

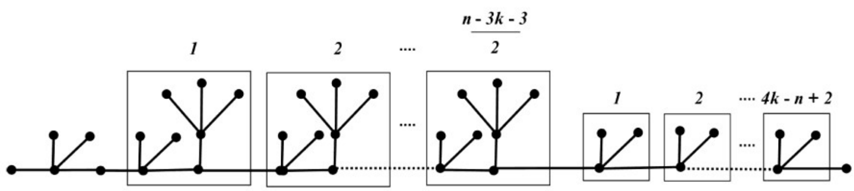


Figure 2
$\boldsymbol{T \in \mathcal{C}_1\mathcal{T}_{n,k}}$ **when** $\boldsymbol{n-k}$ **is odd.**

Corollary 3.3: *If $T \in \mathcal{C}_2\mathcal{T}_{n,k}$ and $n-k$ is even, then the tree T with maximum SO index and minimum harmonic index is shown in Fig. 3.*

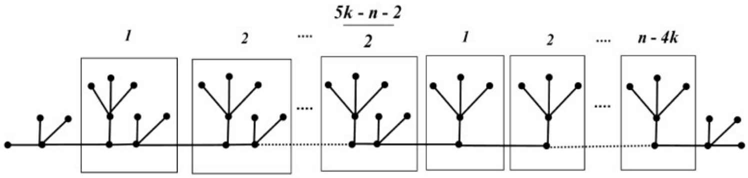


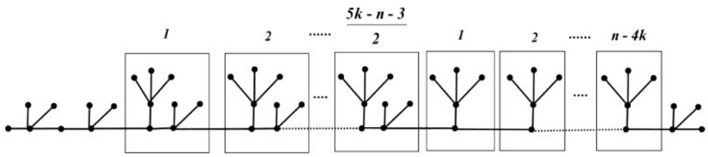
Figure 3

$\boldsymbol{T \in \mathcal{C}_2\mathcal{T}_{n,k}}$ **when** $\boldsymbol{n-k}$ **is even.**

Corollary 3.4: (a) *If* $T \in \mathcal{C}_2\mathcal{T}_{n,k}$, $n-k$ *is odd,* $n=9$ *and* $k=2$, *then the tree* T *with maximum Sombor index and minimum harmonic index is shown in Fig.4a.*

(b) *If* $T \in \mathcal{C}_2\mathcal{T}_{n,k}$, $n-k$ *is odd and* $k \geq 2$, *then the tree* T *with maximum* SO *index and minimum harmonic index is shown in Fig. 4b.*

(a) $\boldsymbol{n=9}$ **and** $\boldsymbol{k=2}$**.**



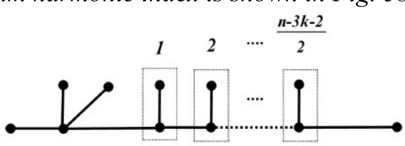
(b) If $\boldsymbol{k \geq 3}$**.**

Figure 4

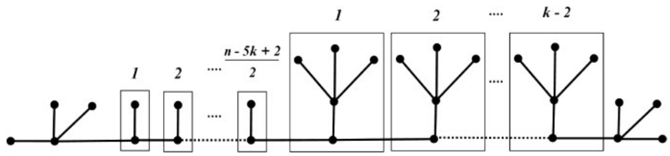
$\boldsymbol{T \in \mathcal{C}_2\mathcal{T}_{n,k}}$ **when** $\boldsymbol{n-k}$ **is odd.**

Corollary 3.5: (a) *If* $T \in \mathcal{C}_3\mathcal{T}_{n,k}$, $n-k$ *is even and* $k=1$, *then the tree* T *with maximum* SO *index and minimum harmonic index is shown in Fig. 5a.*

(b) *If* $T \in \mathcal{C}_3\mathcal{T}_{n,k}$, $n-k$ *is even and* $k \geq 2$, *then the tree* T *with maximum* SO *index and minimum harmonic index is shown in Fig. 5b.*



(a) If $\boldsymbol{k=1}$



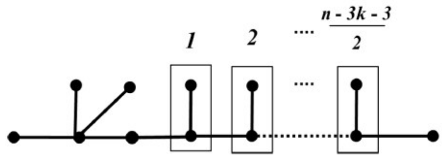
(b) If $\boldsymbol{k \geq 2}$

Figure 5

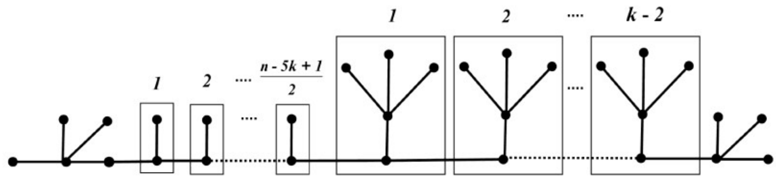
$\boldsymbol{T \in \mathcal{C}_3\mathcal{T}_{n,k}}$ **when** $\boldsymbol{n-k}$ **is even.**

Corollary 3.6: (a) *If $T \in \mathcal{C}_3\mathcal{T}_{n,k}$, $n-k$ is odd and $k=1$, then the tree T with maximum SO index and minimum harmonic index is shown in Fig.6a .*

(b) *If $T \in \mathcal{C}_3\mathcal{T}_{n,k}$, $n-k$ is odd and $k \geq 2$, then the tree T with maximum SO index and minimum harmonic index is shown in Fig. 6b.*



(a) If $k=1$



(b) If $k \geq 2$

Figure 6

$\mathcal{C}_3\mathcal{T}_{n,k}$ when $n-k$ is odd.

4. Conclusion

In this paper, we successfully found extremal chemical trees in $\mathcal{CT}_{n,k}$ that maximize the Sombor index and the same trees simultaneously minimize the harmonic index. Furthermore, we completely characterize and construct the corresponding extremal trees. It is noteworthy that this problem has been addressed for chemical trees. Consequently, we present the following open problem:

Problem 4.1: Find the n-vertex trees with given number of vertices of maximum degree that has maximum Sombor index and minimum harmonic index.

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