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Research article

Maximizing chemical trees of some vertex-degree-based topological indices with given number of pendant vertices

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Abstract: A general VDB topological index of G is defined as

$$\mathcal{TI}_f(G) = \sum_{v_i v_j \in E(G)} f(d_i, d_j),$$

where $f(d_i, d_j)$ is a symmetric function, and d_i represents the degree of $v_i \in V(G)$. This paper aims to address the maximum chemical tree problem for general vertex-degree-based topological indices with given number of pendant vertices via a unified method. Sufficient conditions for general VDB topological indices to take their maximum value are presented, and as an application, we show that there are six VDB topological indices, including the reciprocal sum-connectivity index, the Sombor index, and the Euler Sombor index, etc., that satisfy these conditions.

Keywords: topological indices; chemical trees; extremal trees; pendant vertices
Mathematics Subject Classification: 05C05, 05C09, 05C92

1. Introduction

All graphs involved in this paper are connected, simple, and undirected. Let $G = (V(G), E(G))$ be a graph with vertex set $V(G)$ and edge set $E(G)$. We use $|V(G)| = n$ and $|E(G)| = m$ to represent the total number of edges and vertices in G, respectively. If $m = n - 1$, then G is called a tree, which is generally represented by T.

In the field of chemical mathematics, the molecular structure of a compound is represented by a graph: each atom is represented by a vertex, and the bonds between atoms are signified by the edges between vertices, resulting in a graph called a molecular graph. The graph invariants of molecular graphs are called topological indices. Since Wiener [1] proposed the concept of the Wiener index in 1970, theoretical chemists have used topological indices to quantify molecular information. They are used to represent and predict the physicochemical properties, bioactivities, etc., of chemical compounds [2, 3]. A great number of indices have been generated and studied in mathematics and chemistry [4, 5]. Undoubtedly, the vertex-degree-based (VDB) topological indices are currently the most interesting and extensively investigated [6, 7].

A general VDB topological index of G using the formula

$$\mathcal{TI}_f = \mathcal{TI}_f(G) = \sum_{v_iv_j \in E(G)} f(d_i, d_j),$$

where d_i and d_i refer to the degrees of vertices v_i and v_j respectively, and $f(d_i, d_j)$ is a symmetric function with $d_i, d_j \geq 1$. Let m_{ij} be the number of edges with $(d_i, d_j) = (i, j)$, then

$$\mathcal{TI}_f = \mathcal{TI}_f(G) = \sum_{1 \leq i \leq j \leq \Delta} m_{ij} f(i, j), \tag{1}$$

where Δ signifies the maximal degree of graph G.

As a type of VDB indices originating from geometry [8], the Sombor index is formulated as

$$SO(G) = \sum_{v_iv_j \in E(G)} \sqrt{d_i^2 + d_j^2},$$

and it has received increasing attention since its proposal. Maitreyi et al. [9] established the minimal Sombor index for trees with fixed pendant vertices. Liu et al. [10] identified the maximal Sombor index of chemical trees having a given number of even pendants. In 2022, Chen et al. [11] determined the extremal values on the Sombor index of trees with given parameters such as diameter, pendant vertices, segment number, etc. Chen and Zhu [12] attained the maximum and minimum Sombor index of chemical unicyclic graphs with a given girth. Cruz and Rada [13] investigated the extremal unicyclic and bicyclic graphs with the Sombor index but did not characterize the extremal graphs. In 2024, Das [14] completely solved these problems. Liu et al. [15] ordered the minimum Sombor indices for chemical unicyclic graphs, chemical bicyclic graphs, and chemical tricyclic graphs. In addition, it also involves related research on c-cyclic graphs [16], their chemical properties and applications [17, 18], and other aspects [19, 20].

In [21], the general Sombor index is labeled as

$$SO_\alpha(G) = \sum_{v_iv_j \in E(G)} (d_i^2 + d_j^2)^\alpha,$$

where $\alpha \neq 0$ is an appropriate selectable exponent. Maitreyi et al. [22] explored the general Sombor index of trees with given pendents for $0 < \alpha < 1$. Very recently, Ahmad and Das [23] have completely solved the maximal general Sombor index for chemical trees with given number of pendant vertices, where $\alpha \in (0.144, 3.335)$.

Exploring a universal method applicable to various topological indices has long been a key issue that scholars have explored. In 2021, Brezovnik and Tratnik [24] introduced the concept of a general Szeged-like topological index for various distance-based topological indices and proposed a cutting method to calculate this index for any strength-weighted graph. These results were also applied to benzenoid systems, phenylenes, and coronoid systems, which are well-known families of molecular graphs. Moreover, Gao [25] uses a universal method to solve the extremal problems with general VDB topological indices for c-cyclic graphs and shows that if the VDB topological index satisfies such conditions for $f(x, y)$, then the corresponding extremal graphs have been determined.

Inspired by [24] and [25], we use a unified method to explore the extremum VDB indices for chemical trees with given number of pendant vertices. In Sections 2 and 3, we introduce the notations, terminology, and several lemmas used throughout the article. Building on these lemmas, in Section 4, we establish sufficient conditions for chemical trees of order n and pendant number k (whose collection is denoted by $\mathcal{CT}_{n,k}$) that achieve the maximum VDB topological index and further characterize the corresponding extremal graphs. In Section 5, as an application, we show that six VDB topological indices, including the reciprocal sum-connectivity index, the Euler Sombor index, among others, satisfy the conditions established in Section 4 and attain their maximum values on the chemical trees $\mathcal{CT}_{n,k}$. In the final Section 6, we summarize the paper and outline directions for future work.

2. Notations and terminologies

In this section, we introduce some definitions and terms of trees used in this article. For any vertex v_i in tree T, the (open) neighborhood N_i is defined as the set of all vertices adjacent to v_i. If the number of neighborhoods $|N_i| \leq 4$ for all vertices, then T is called a chemical tree. A vertex v is a pendant vertex if $d_v = 1$, while the vertex with degree at least three is called the branching vertex in the tree. For any $v_iv_j \in E(T)$, we use $T - v_iv_j$ to represent the obtained graph by removing the edge $v_iv_j \in T$, and we use $T + v_iv_j$ to denote the resulting graph by connecting the edge $v_iv_j \notin E(T)$.

The degree sequence of T, denoted by $D(T) = (d_1, d_2, \cdots, d_{n-1})$, is a sequence of degrees of its vertices, where $d_1 > d_2 > \cdots > d_{n-1}$. Let $P(i, j) = v_1v_2 \cdots v_q$ denote the path of T with two end vertices v_1 and v_q, where $d_1 = i$, $d_2 = \cdots = d_{q-1} = 2$, and $d_q = j$. In particular, $P(i, j)$ signifies the internal path if $d_1 = i \geq 3$ and $d_q = j \geq 3$. And also, $|P(i, j)|$ represents the length of such a path $P(i, j)$. Notice that if two end vertices satisfy that $d_1 = 1$ and $d_q = 1$, then T is called a path labeled as P_n. Similarly, the star is denoted by S_n, if there is a central vertex v_n such that $d_n = n - 1$, and all other vertices v_i with $d_i = 1$ (where $1 \leq i \leq n - 1$). Other terms and definitions not introduced herein refer to [24].

For convenience, we denote the collection of the chemical trees with order n as $\mathcal{CT}_n$, while the collection of the chemical trees with order n and k pendant vertices simultaneously is denoted by $\mathcal{CT}_{n,k}$. As we know, each (chemical) tree has at least two pendant vertices, so $n \geq k + 2$. The collection of maximal chemical trees in $\mathcal{CT}_{n,k}$, is defined as follows:

$$\mathcal{CT}_{n,k}^{max} = \{T \in \mathcal{CT}_{n,k} : \ TI_f(T) \text{ attains its maximum value}\}.$$

Recall that d_i represents the degree of $v_i \in V(G)$, and m_{ij} is the total number of edges with $(d_i, d_j) = (i, j)$. In this paper, we use n_i to signify the number of vertices in T with degree i. Therefore, for any $T \in \mathcal{CT}_{n,k}$ and $1 \leq i \leq 4$, the following relations hold:

$$\begin{cases} k + n_2 + n_3 + n_4 = n, \\ k + 2n_2 + 3n_3 + 4n_4 = 2n - 2, \\ i \cdot n_i = 2m_{ii} + \sum\limits_{1 \le j \le 4}^{j \ne i} m_{ij}, \text{ where } 1 \le i \le 4. \end{cases} \tag{2}$$

3. Some lemmas

Lemma 3.1. *(Ahmad and Das [23]) Let $T \in \mathcal{CT}_{n,k}$, then*

(i) $n_3 = 0$ if and only if T has the degree sequence $\pi_1(T) = (\underbrace{4, \cdots, 4}_{\frac{k-2}{2}}, \underbrace{2, \cdots, 2}_{\frac{2n-3k+2}{2}}, \underbrace{1, \cdots, 1}_{k})$.

(ii) $n_3 = 1$ if and only if T has the degree sequence $\pi_2(T) = (\underbrace{4, \cdots, 4}_{\frac{k-3}{2}}, 3, \underbrace{2, \cdots, 2}_{\frac{2n-3k+1}{2}}, \underbrace{1, \cdots, 1}_{k})$.

Lemma 3.2. *Let $1 \le r < s \le 4$ and $1 \le x \le 4$. If $g(x) = f(x, s) - f(x, r)$ is strictly decreasing with respect to x, and the following two conditions hold:*

(i) $3(f(4, 4) - f(3, 4)) + f(2, 4) - f(3, 3) + f(1, 2) - f(1, 3) > 0$*, and*

(ii) $4(f(4, 4) - f(3, 4)) + f(2, 2) - f(2, 3) + f(1, 2) - f(1, 3) > 0$.

Then $T \in \mathcal{CT}_{n,k}^{max}$ contains at most one vertex with degree 3.

Proof. Assume T contains two vertices, v_i and v_j with degrees of 3, and let $N_i(T) = \{v_1, v_2, v_3\}$, $N_j(T) = \{v_{1'}, v_{2'}, v_{3'}\}$. Without loss of generality, let v_3 and $v_{3'}$ lie on the $v_i - v_j$ path, where v_j or $v_{3'}$ may be the same as v_3. Because $v_3 \in N_i(T)$ and $v_{3'} \in N_j(T)$ are located on the $v_i - v_j$ path, they have $2 \le d_3, d_{3'} \le 4$ and $1 \le d_1, d_2, d_{1'}, d_{2'} \le 4$. Now, we construct the following useful transformation.

Transformation 1: $T_1 = T - v_j v_{2'} + v_{2'} v_i$.

Notice that $T_1 \in \mathcal{CT}_{n,k}$, $d_i(T_1) = 4$, and $d_j(T_1) = 2$; the degrees of other vertices remain unchanged. We consider two cases based on whether $v_i v_j \in E(T)$ or $v_i v_j \notin E(T)$.

Case 1. $v_i v_j \in E(T)$. Then $v_j = v_3$ or $v_{3'} = v_i$. Due to Transformation 1, we have

$$\begin{aligned} TI_f(T_1) - TI_f(T) = {} & f(d_1, 4) - f(d_1, 3) + f(d_2, 4) - f(d_2, 3) + f(2, 4) - f(3, 3) \\ & + f(d_{2'}, 4) - f(d_{2'}, 3) + f(d_{1'}, 2) - f(d_{1'}, 3). \end{aligned}$$

Given that $g(x)$ is strictly decreasing with respect to x, and the condition (i), we deduce

$$TI_f(T_1) - TI_f(T) \ge 3(f(4, 4) - f(3, 4)) + f(2, 4) - f(3, 3) + f(1, 2) - f(1, 3) > 0.$$

Hence $TI_f(T_1) > TI_f(T)$, this contradicts our assumption that $T \in \mathcal{CT}_{n,k}^{max}$.

Case 2. $v_i v_j \notin E(T)$. No matter if $v_3 = v_{3'}$ or $v_3 \ne v_{3'}$, according to Transformation 1, we obtain

$$\begin{aligned} TI_f(T_1) - TI_f(T) = {} & f(d_1, 4) - f(d_1, 3) + f(d_2, 4) - f(d_2, 3) + f(d_3, 4) - f(d_3, 3) \\ & + f(d_{2'}, 4) - f(d_{2'}, 3) + f(d_{1'}, 2) - f(d_{1'}, 3) + f(d_{3'}, 2) - f(d_{3'}, 3). \end{aligned}$$

Given that $g(x)$ is strictly decreasing with respect to x and the condition (ii), we obtain

$$TI_f(T_1) - TI_f(T) \ge 4(f(4, 4) - f(3, 4)) + f(2, 2) - f(2, 3) + f(1, 2) - f(1, 3) > 0,$$

which means $TI_f(T_1) > TI_f(T)$, this contradicts $T \in \mathcal{CT}_{n,k}^{max}$. Consequently, the hypothesis is not valid, and the proof is complete. □

Recall that $P(i, j)$ is the path with two end vertices that have degrees i and j, respectively, while its internal vertices have degree 2. For the convenience of subsequent results, we define several sets of trees as follows.

Let $A_1 = \{T \in \mathcal{CT}_{n,k}^{max} : |P(i,1)| = 1 \text{ for all } P(i,1) \in P(T), \text{ where } 3 \leq i \leq 4\}$.

Let $A_2 = \{T \in \mathcal{CT}_{n,k}^{max}$: for $3 \leq i \leq 4$, either $|P(4,i)| \leq 2$ for all $P(4,i) \in P(T)$, or $|P(4,i)| \geq 2$ for all $P(4,i) \in P(T)\}$.

Let $B_1 = \{T \in \mathcal{CT}_{n,k}^{max} : n_3(T) = 1$, either $v_iv_j \notin E(T)$ for $d_i = 3$ and $d_j = 1$, or $P(4,4) \notin P(T)\}$.

Let $B_2 = \{T \in \mathcal{CT}_{n,k}^{max} : n_3(T) = 1$, either $v_iv_j \notin E(T)$ for $d_i = d_j = 4$, or $|P(3,4)| = 1$ for all $P(3,4) \in P(T)\}$.

Lemma 3.3. *Let $T \in \mathcal{CT}_{n,k}^{max}$, $k \geq 5$. If $g(x) = f(x,s) - f(x,r)$ is strictly decreasing with respect to x, where $1 \leq r < s \leq 4$, $1 \leq x \leq 4$, then $T \in A_1$ and $T \in A_2$.*

Proof. First, prove $T \in A_1$. Assuming the contrary, that $T \notin A_1$, and hence T contains a pendant path $P(i,1) = v_1v_2\cdots v_l (l \geq 3)$, where $d_1 = 3,4$, and $d_l = 1$. Due to $k \geq 5$, T has another branch vertex, let it be $v_q \neq v_1 (d_q \geq 3)$, which produces an internal path $v_1 - v_q$. Suppose $v_{1'}$ is a neighborhood vertex of v_1 except for v_2 located in the internal path of $v_1 - v_q$, where maybe $v_{1'} = v_q$. Now, we construct the following transformation.

Transformation 2: $T_2 = T - \{v_1v_{1'}, v_{l-1}v_l\} + \{v_1v_l, v_{1'}v_{l-1}\}$.

Then $T_2 \in \mathcal{CT}_{n,k}$, and $d_j(T_2) = d_j(T)$ for all v_j in T. Regardless of whether $v_{1'}$ is the same as v_q, by Transformation 2, we obtain

$$TI_f(T_2) - TI_f(T) = f(1,d_1) - f(1,2) + f(d_{1'},2) - f(d_{1'},d_1),$$

where $3 \leq d_1 \leq 4$, $2 \leq d_{1'} \leq 4$. Since $g(x)$ is strictly decreasing, and thus $g(1) = f(1,d_1) - f(1,2) > f(d_{1'},d_1) - f(d_{1'},2) = g(d_{1'}) \leq g(2)$. Therefore, we deduce

$$TI_f(T_2) - TI_f(T) = f(d_1,1) - f(2,1) + f(d_{1'},2) - f(d_1,d_{1'}) > 0,$$

which contradicts $T \in \mathcal{CT}_{n,k}^{max}$. So, the assumption $T \notin A_1$ is not true, and thus $T \in A_1$.

Now prove $T \in A_2$. Assume $T \notin A_2$; then T contains two internal paths, $P(4,j) = v_1v_2\cdots v_l (l \geq 4)$ and $P'(4,j) = v_{1'}v_{2'}$, where $d_1 = d_{1'} = 4$, and $d_l = d_{2'} \geq 3$.

Transformation 3: $T_3 = T - \{v_1v_2, v_2v_3, v_{1'}v_{2'}\} + \{v_1v_3, v_{1'}v_2, v_2v_{2'}\}$.

Then $T_3 \in \mathcal{CT}_{n,k}$, and $d_j(T_3) = d_j(T)$ for all vertex v_j in T. Whether $v_{1'}$ is the same as $v_{2'}$ or v_l, by Transformation 3, we have

$$TI_f(T_3) - TI_f(T) = f(d_{2'},2) - f(d_{2'},4) + f(2,4) - f(2,2).$$

Since $g(x)$ is strictly decreasing, and $3 \leq d_{2'} \leq 4$, we obtain $g(2) = f(2,4) - f(2,2) > f(d_{2'},4) - f(d_{2'},2) = g(d_{2'}) \leq g(3)$. Consequently,

$$TI_f(T_3) - TI_f(T) = f(d_{2'},2) - f(d_{2'},4) + f(2,4) - f(2,2) > 0,$$

which contradicts $T \in \mathcal{CT}_{n,k}^{max}$. Therefore, $T \in A_2$, and the proof is done. □

Lemma 3.4. *Let $T \in \mathcal{CT}_{n,k}^{max}$, $k \geq 5$, and $n_3 = 1$. If $g(x) = f(x,s) - f(x,r)$ is strictly decreasing with respect to x, where $1 \leq r < s \leq 4$, $1 \leq x \leq 4$, then $T \in B_1$ and $T \in B_2$.*

Proof. First, prove $T \in B_1$. For $k = 5$, then $n_4 = \frac{k-3}{2} = 1$. According to the definition of B_1, it is clear that $T \in B_1$.

Next, assume $k \geq 6$; then $n_4 \geq 2$. Suppose for contradiction that $T \notin B_1$, then T contains an internal path $P(4,4) = v_1v_2 \cdots v_l (l \geq 2)$ and with an edge $v_iv_j \in E(T)$, where $d_1 = d_l = 4$, $d_i = 3$, and $d_j = 1$. Without loss of generality, suppose v_1 is placed in the $v_i - v_l$ path.

Transformation 4: $T_4 = T - \{v_1v_2, v_iv_j\} + \{v_1v_j, v_2v_i\}$.

Then $T_4 \in \mathcal{CT}_{n,k}$, and $d_t(T_4) = d_t(T)$ for all vertex v_t in T. Now, we will discuss two cases according to the values of $|P(4,4)|$.

Case 1. $|P(4,4)| = 1$. Thus, $l = 2$. By Transformation 4, we have

$$TI_f(T_4) - TI_f(T) = f(1,4) - f(1,3) + f(3,4) - f(4,4).$$

Since $g(x)$ is strictly decreasing, we have $g(1) = f(1,4) - f(1,3) > f(4,4) - f(4,3) = g(4)$, and hence $TI_f(T_4) > TI_f(T)$; this contradicts $T \in \mathcal{CT}_{n,k}^{max}$. So the assumption $T \notin B_1$ is not true, and thus $T \in B_1$.

Case 2. $|P(4,4)| > 1$. In this case, $l \geq 3$, and hence,

$$TI_f(T_4) - TI_f(T) = f(1,4) - f(1,3) + f(2,3) - f(2,4).$$

Similarly to the proof of Case 1, we deduce that $TI_f(T_4) > TI_f(T)$, which contradicts $T \in \mathcal{CT}_{n,k}^{max}$. Therefore, $T \in B_1$.

Next, we prove $T \in B_2$. For $k = 5$, have $n_4 = 1$. By the definition of B_2, $T \in B_2$ is established.

In the following, we assume that $k \geq 6$, and in this case, $n_4 \geq 2$. Assume the opposite, that $T \notin B_2$; then T has an edge $v_iv_j \in E(T)$, such that $d_i = d_j = 4$, and contains an internal path $P(4,3) = v_1v_2 \cdots v_l (l \geq 3)$, where $d_1 = 4$, $d_l = 3$, and v_1 may coincide with v_i or v_j.

Transformation 5: $T_5 = T - \{v_1v_2, v_2v_3, v_iv_j\} + \{v_1v_3, v_2v_i, v_2v_j\}$.

Then $T_5 \in \mathcal{CT}_{n,k}$, and the degrees of all vertices in T_5 and T remain unchanged. Now, we will discuss two cases based on the value of $|P(3,4)|$.

Case 1. $|P(3,4)| = 2$. Then $l = 3$, and Transformation 5 implies that

$$TI_f(T_5) - TI_f(T) = f(2,4) - f(2,3) + f(4,3) - f(4,4).$$

Since $g(x)$ is strictly decreasing, we have $g(2) = f(2,4) - f(2,3) > f(4,4) - f(4,3) = g(4)$, and hence $TI_f(T_5) > TI_f(T)$, which contradicts $T \in \mathcal{CT}_{n,k}^{max}$. Consequently, the assumption $T \notin B_2$ does not hold, and thus $T \in B_2$.

Case 2. $|P(3,4)| > 2$. Then $l > 3$. Analogously to Case 1, we derive

$$TI_f(T_5) - TI_f(T) = f(2,4) - f(2,2) + f(4,2) - f(4,4).$$

Since $g(x)$ is strictly decreasing, we have $g(2) = f(2,4) - f(2,2) > f(4,4) - f(4,2) = g(4)$, and thus $TI_f(T_5) > TI_f(T)$; this contradicts $T \in \mathcal{CT}_{n,k}^{max}$. So, $T \in B_2$.

Therefore, based on the above cases, the lemma is proven. □

4. Maximal VDB topological indices among $\mathcal{CT}_{n,k}$

In this section, we determine the maximum VDB topological indices over $\mathcal{CT}_{n,k}$, and characterize the graphs that attain these maximum values.

We denote the broom tree as $\mathcal{B}_{n,k}$, which is obtained by coalescing the central vertex of the star S_k with a pendant vertex of the path P_{n-k}. Clearly, there is only one path $P(k,1) \in P(T)$, such that $|P(k,1)| \geq 2$.

Theorem 4.1. *Let $T \in \mathcal{CT}_{n,k}$ with $3 \leq k \leq 4$ and $n \geq k+2$. If $g(x) = f(x,s) - f(x,r)$ is strictly decreasing with respect to x, where $1 \leq r < s \leq 2$, and $2 \leq x \leq 4$. Then*

$$TI_f(T) \leq (k-1)f(1,k) + f(1,2) + (n-k-2)f(2,2) + f(2,k),$$

the equality occurs if and only if $T \cong \mathcal{B}_{n,k}$.

Proof. Let $T^* \in \mathcal{CT}_{n,k}^{max}$, and assume for contradiction that $T^* \ncong \mathcal{B}_{n,k}$. Thus, there exist two paths $P(k,1) \in P(T)$ $(k = 3, 4)$, such that $|P(k,1)| \geq 2$. Without loss of generality, let $P_1(k,1) = v_1 v_2 \cdots v_l (l \geq 3)$, and $P_2(k,1) = u_1 u_2 \cdots u_q (q \geq 3)$. By Lemma 3.1, when $k = 3$ and $k = 4$, T^* has the following degree sequences, respectively:

$$\pi_3(T^*) = (3, \underbrace{2, \cdots, 2}_{n-4}, 1, 1, 1), \text{ and } \pi_4(T^*) = (4, \underbrace{2, \cdots, 2}_{n-5}, 1, 1, 1, 1).$$

Since there is only one vertex with a degree greater than or equal to 3, this implies that $u_1 = v_1$.
Transformation 6: $T_6 = T^* - v_2 v_3 + u_q v_3$.

Then $T_6 \in \mathcal{CT}_{n,k}$, $d_{v_2}(T_6) = 1$, $d_{v_2}(T^*) = 2$, $d_{v_i}(T_6) = d_{v_i}(T)$, and $d_{u_j}(T_6) = d_{u_j}(T^*)$ for all other $v_i, u_j \in T^*$. According to Transformation 6, we obtain

$$TI_f(T_6) - TI_f(T^*) = f(k,1) - f(k,2) + f(2,2) - f(2,1),$$

where $k = 3$ and 4. Since $g(x)$ is strictly decreasing, we have $g(2) = f(2,2) - f(2,1) > f(k,2) - f(k,1) = g(k)$, and hence,

$$TI_f(T_6) - TI_f(T^*) = f(k,1) - f(k,2) + f(2,2) - f(2,1) > 0.$$

That is, $TI_f(T_6) > TI_f(T^*)$, which contradicts $T^* \in \mathcal{CT}_{n,k}^{max}$. So, the assumption $T^* \ncong \mathcal{B}_{n,k}$ does not hold, and thus $T^* \cong \mathcal{B}_{n,k}$. In this case, $m_{1k} = k-1$, $m_{12} = m_{2k} = 1$, and $m_{22} = (n-k-2)$. Consequently, by the relation (1), we have

$$TI_f(T^*) = (k-1)f(1,k) + f(1,2) + (n-k-2)f(2,2) + f(2,k),$$

the equality occurs if and only if $T^* \cong \mathcal{B}_{n,k}$, and this establishes the result. □

Before presenting the following main theorem, we define two sets of trees as follows:
$\mathcal{CT}^1 = \{T \in \mathcal{CT}_{n,k}^{max} : k \geq 6 \textit{ is even}, D(T) = \pi_1(T), \textit{and } T \in A_1 \cap A_2\}$.
$\mathcal{CT}^2 = \{T \in \mathcal{CT}_{n,k}^{max} : k \geq 5 \textit{ is odd}, D(T) = \pi_2(T), \textit{and } T \in A_1 \cap A_2 \cap B_1 \cap B_2\}$.

Theorem 4.2. *Let $T \in \mathcal{CT}_{n,k}$ with $k \geq 5$ and $n \geq k+2$. Suppose $g(x) = f(x,s) - f(x,r)$ is strictly decreasing with respect to x, where $1 \leq r < s \leq 4$, and $1 \leq x \leq 4$. If the following conditions hold:*

(i) $3(f(4,4) - f(3,4)) + f(2,4) - f(3,3) + f(1,2) - f(1,3) > 0$, *and*

(ii) $4(f(4,4) - f(3,4)) + f(2,2) - f(2,3) + f(1,2) - f(1,3) > 0$.

Then, we have the following conclusions:

(I) If $k \geq 6$ is even, then

$$TI_f(T) \leq \begin{cases} kf(1,4) + (2n-3k+2)f(2,4) + (2k-n-3)f(4,4), & n \leq 2k-4, \\ kf(1,4) + (k-4)f(2,4) + (n-2k+3)f(2,2), & n \geq 2k-3, \end{cases}$$

the equality occurs if and only if $T \in \mathcal{CT}^1$.

(II) If $k \geq 5$ is odd, then

$$TI_f(T) \leq \begin{cases} 2f(1,3) + 3f(1,4) + f(3,4), & k=5, n=7, \\ 2f(1,3) + 3f(1,4) + f(2,3) + f(2,4) + (n-8)f(2,2), & k=5, n \geq 8, \\ f(1,3) + 6f(1,4) + (n-10)(f(2,3) + f(2,4)) + (12-n)f(3,4), & k=7, n=10,11, \\ f(1,3) + 6f(1,4) + 2(f(2,3) + f(2,4)) + (n-12)f(2,2), & k=7, n \geq 12, \\ 9f(1,4) + (n-13)(f(2,3) + f(2,4)) + (16-n)f(3,4), & k=9, 13 \leq n \leq 15, \\ 9f(1,4) + 3(f(2,3) + f(2,4)) + (n-16)f(2,2), & k=9, n \geq 16, \\ kf(1,4) + 3f(3,4) + (2n-3k+1)f(2,4) + (2k-n-5)f(4,4), & \\ \qquad k \geq 11, 16 \leq n \leq 2k-6, & \\ kf(1,4) + (n-2k+5)f(2,3) + (2k-n-2)f(3,4) + (n-k-4)f(2,4), & \\ \qquad k \geq 11, 2k-5 \leq n \leq 2k-3, & \\ kf(1,4) + 3f(2,3) + (k-6)f(2,4) + (n-2k+2)f(2,2), & \\ \qquad k \geq 11, n \geq 2k-2, & \end{cases}$$

the equality occurs if and only if $T \in \mathcal{CT}^2$.

Proof. Let T^* be the maximum chemical tree of TI_f, then $TI_f(T) \leq TI_f(T^*)$. The equality occurs if and only if $T \cong T^*$. Furthermore, $T^* \in \mathcal{CT}^{max}_{n,k}$. Next, we will determine the value of $TI_f(T^*)$. According to Lemma 3.2, $n_3 \leq 1$. Moreover, by Lemma 3.1, if $n_3 = 0$, we have

$$\pi_1(T^*) = (\underbrace{4, \cdots, 4}_{\frac{k-2}{2}}, \underbrace{2, \cdots, 2}_{\frac{2n-3k+2}{2}}, \underbrace{1, \cdots, 1}_{k}).$$

Thus, k is even. If $n_3 = 1$, we have

$$\pi_2(T^*) = (\underbrace{4, \cdots, 4}_{\frac{k-3}{2}}, 3, \underbrace{2, \cdots, 2}_{\frac{2n-3k+1}{2}}, \underbrace{1, \cdots, 1}_{k}).$$

Then, k is odd. Next, we will consider two cases based on the parity of k.

(I) k is even. And hence $k \geq 6$. By Lemma 3.3, $T^* \in A_1 \cap A_2$, and hence $T^* \in \mathcal{CT}^1$. Because of $n_3 = 0$ and $T^* \in A_1$, then $|P(4,1)| = 1$ for all paths $P(4,1) \in P(T^*)$. Therefore, $m_{12} = 0$, and $m_{14} = n_1 = k$. This, together with $n_3 = 0$, implies that $m_{13} = m_{23} = m_{33} = m_{43} = 0$. By substituting these into relation (2), we deduce that

$$m_{14} = k, \;\; 2m_{22} + m_{24} = 2n - 3k + 2, \;\; m_{24} + 2m_{44} = k - 4. \tag{3}$$

The discussion is partitioned into two cases depending on the value of n.

Case 1. $n \le 2k-4$. Then $n_2 = \frac{2n-3k+2}{2} < \frac{k-4}{2} = n_4 - 1$. If $m_{22} \ge 1$, by the known facts that $n_3 = 0$ and $m_{12} = 0$, there exists a path $P(4,4)$, such that $|P(4,4)| \ge 3$. According to $T^* \in A_2$, then $|P(4,4)| \ge 2$ for all $P(4,4) \in P(T^*)$. In this case, we deduce that $n_2 > n_4 - 1$, which contradicts $n_2 < n_4 - 1$. Therefore, we have $m_{22} = 0$. It can be concluded from (3) that $m_{24} = 2n - 3k + 2$, $m_{44} = 2k - n - 3$. Consequently, we deduce from (1) that

$$TI_f(T^*) = kf(1,4) + (2n-3k+2)f(2,4) + (2k-n-3)f(4,4).$$

Case 2. $n \ge 2k-3$. Then $n_2 = \frac{2n-3k+2}{2} \ge \frac{k-4}{2} = n_4 - 1$. If $m_{44} \ge 1$, there exists a path $P(4,4)$, such that $|P(4,4)| = 1$. Since $T^* \in A_2$, then $|P(4,4)| \le 2$ for all $P(4,4) \in P(T^*)$. This yields $n_2 < n_4 - 1$, which contradicts $n_2 \ge n_4 - 1$. So, $m_{44} = 0$. We can conclude from (3) that $m_{22} = n - 2k + 3$, $m_{24} = k - 4$. Therefore, we obtain

$$TI_f(T^*) = kf(1,4) + (k-4)f(2,4) + (n-2k+3)f(2,2).$$

So, the case n is even has been achieved.

(II) k is odd. And thus $k \ge 5$. In this case, $n_3 = 1$ and $m_{33} = 0$. By applying Lemma 3.3 and 3.4, we deduce that $T^* \in A_1 \cap A_2 \cap B_1 \cap B_2$. That is, $T^* \in \mathcal{CT}^2$. As $n_3 = 1$ and $T^* \in A_1$, this yields that for $3 \le i \le 4$, $|P(i,1)| = 1$ for all $P(i,1) \in P(T^*)$. Hence, $m_{12} = 0$. Therefore, by substituting these results into (2), we have the following relation:

$$m_{13} + m_{14} = k, \;\; 2m_{22} + m_{23} + m_{24} = 2n - 3k + 1,$$

$$m_{13} + m_{23} + m_{34} = 3, \;\; m_{14} + m_{24} + m_{34} + 2m_{44} = 2k - 6. \tag{4}$$

Let $v \in T^*$, and $d_v(T^*) = 3$. Next, we will discuss two cases.

Case 1. $k = 5$. Then $n_4 = 1$. If $n = 7$, the collection $\mathcal{CT}_{7,5}$ contains a unique tree, where $\pi_2(T^*) = (4,3,1,1,1,1,1)$, together with (4), we deduce that $m_{13} = 2$, $m_{14} = 3$, and $m_{34} = 1$. Consequently,

$$TI_f(T^*) = 2f(1,3) + 3f(1,4) + f(3,4).$$

If $n \ge 8$, as $n_3 = 1$ and $m_{12} = 0$, together with (4), we deduce $m_{13} = 2$, $m_{14} = 3$, $m_{23} = m_{24} = 1$, $m_{34} = 0$, and $m_{22} = n - 8$. Therefore, we have

$$TI_f(T^*) = 2f(1,3) + 3f(1,4) + f(2,3) + f(2,4) + (n-8)f(2,2).$$

Case 2. $k = 7$. Then $n \ge 10$, and $n_4 = 2$. According to $m_{12} = 0$, there is at least one pendant vertex connecting to the vertex of degree 3, i.e., $m_{13} \ge 1$.

If $m_{13} \ge 2$, then $P(4,4) \in P(T^*)$, which contradicts $T^* \in B_1$. Therefore, $m_{13} = 1$. Together with $n_4 = 2$ and relation (4), this implies that $m_{14} = 6$, $m_{44} = 0$, and $m_{13} = 1$. In this case, we deduce that

$$2m_{22} + m_{23} + m_{24} = 2n - 20, \;\; m_{23} + m_{34} = 2, \;\; m_{24} + m_{34} = 2. \tag{5}$$

Case 2.1. $n = 10$. Now, applying relation (5), have $m_{23} = m_{24} = m_{22} = 0$, $m_{34} = 2$. Consequently,

$$TI_f(T^*) = f(1,3) + 6f(1,4) + 2f(3,4).$$

Case 2.2. $n = 11$. The fact that $n_2 = 1$ implies that $m_{22} = 0$. Applying relation (5), we have $m_{23} = m_{24} = m_{34} = 1$. And thus,

$$TI_f(T^*) = f(1,3) + 6f(1,4) + f(2,3) + f(2,4) + f(3,4).$$

Case 2.3. $n \geq 12$. Then $n_2 = \frac{2n-3k+1}{2} \geq 2$. If $m_{34} = 1$, there exists a path $P(4,3) \in P(T^*)$, having $|P(4,3)| = 1$. Since $T^* \in A_2$, then $|P(4,3)| \leq 2$ for all $P(4,3) \in P(T^*)$. Together with $m_{13} = 1$ and $m_{34} = 1$, this yields that $m_{23} \leq 1$, i.e., $n_2 \leq 1$, which contradicts $n_2 \geq 2$. Therefore, $m_{34} = 0$. Using relation (5), we have $m_{23} = m_{24} = 2$ and $m_{22} = n - 12$. Consequently,

$$TI_f(T^*) = f(1,3) + 6f(1,4) + 2(f(2,3) + f(2,4)) + (n-12)f(2,2).$$

Case 3. $k = 9$. Then $n \geq 13$, and $n_4 = 3$. If $m_{13} \geq 1$, by the known fact $n_3 = 1$, there exists $P(4,4) \in P(T^*)$, which contradicts $T^* \in B_1$. Therefore, $m_{13} = 0$. Similarly, if $m_{44} \geq 1$, there exists $m_{13} \geq 1$, which contradicts $T^* \in B_1$ again. Hence, $m_{44} = 0$. So, using relation (4), we deduce that

$$m_{14} = 9, \;\; 2m_{22} + m_{23} + m_{24} = 2n - 26, \;\; m_{23} + m_{34} = 3, \;\; m_{24} + m_{34} = 3. \tag{6}$$

Case 3.1. $13 \leq n \leq 15$. Then $0 \leq n_2 \leq 2$. By Lemma 3.3, and together with $m_{12} = 0$, $n_4 = 3$, and $n_3 = 1$, it can be concluded that $m_{22} = 0$. Therefore, using the relation (6), we deduce that $m_{23} = m_{24} = n - 13$, $m_{34} = 16 - n$, $m_{14} = 9$. In this case, we have

$$TI_f(T^*) = 9f(1,4) + (n-13)(f(2,3) + f(2,4)) + (16-n)f(3,4).$$

Case 3.2. $n \geq 16$. Then $n_2 \geq 3$. Similar to Case 2.3, it can be concluded from Lemma 3.3 that $m_{34} = 0$. Using relation (6), we deduce $m_{23} = m_{24} = 3$ and $m_{22} = n - 16$. Consequently,

$$TI_f(T^*) = 9f(1,4) + 3(f(2,3) + f(2,4)) + (n-16)f(2,2).$$

Case 4. $k \geq 11$. Then $n_4 \geq 4$ and $n \geq 16$. As $n_3 = 1$, similarly with Case 3, we deduce that $m_{13} = 0$. Otherwise, there will be a contradiction with $T^* \in B_1$.

Case 4.1. $n \leq 2k - 6$. Then $n_2 = \frac{2n-3k+1}{2} \leq \frac{k-11}{2} = n_4 - 4$. As $T^* \in A_2$, either $|P(4,j)| \leq 2$ for all $P(4,j) \in P(T^*)$, or $|P(4,j)| \geq 2$ for all $P(4,j) \in P(T^*)$, where $3 \leq j \leq 4$. The fact that $n_2 \leq n_4 - 4$ implies that $m_{22} = 0$ and $m_{44} \neq 0$. And thus, according to $m_{44} \neq 0$ and $T^* \in B_2$, we obtain $|P(4,3)| = 1$ for all $P(4,3) \in P(T^*)$. Hence, $m_{34} = 3$. Since $m_{13} = 0$, using relation (4), this yields $m_{14} = k$, $m_{44} = 2k - n - 5$, and $m_{24} = 2n - 3k + 1$. Immediately, we have

$$TI_f(T^*) = kf(1,4) + 3f(3,4) + (2n-3k+1)f(2,4) + (2k-n-5)f(4,4).$$

Case 4.2. $2k - 5 \leq n \leq 2k - 3$. Then $n_4 - 3 \leq n_2 = \frac{2n-3k+1}{2} \leq \frac{k-5}{2} = n_4 - 1$. If $m_{44} \geq 1$, then $T^* \in B_2$ implies that $n_2 < n_4 - 3$; this contradicts $n_2 \geq n_4 - 3$. Thus, $m_{44} = 0$. Similarly, if $m_{34} = 0$, then $T^* \in B_2$ implies that $n_2 > n_4 - 1$, which contradicts $n_2 \geq n_4 - 1$. And hence $m_{34} \geq 1$. This, together with $T^* \in A_2$, we deduce that $m_{22} = 0$. Therefore, using relation (4), we obtain $m_{14} = k$, $m_{24} = n - k - 4$, $m_{23} = n - 2k + 5$, and $m_{34} = 2k - 2 - n$. Consequently,

$$TI_f(T^*) = kf(1,4) + (n-2k+5)f(2,3) + (2k-n-2)f(3,4) + (n-k-4)f(2,4).$$

Case 4.3. $n \geq 2k-2$. Then $n_2 \geq n_4$. Since $T^* \in B_2$, similarly to Case 4.2, we deduce $m_{44} = 0$. For the same reason, we can deduce that $m_{34} = 0$. Otherwise, a contradiction can be inferred from $T^* \in A_2$. Therefore, using relation (4), we deduce that $m_{14} = k$, $m_{22} = n-2k+2$, $m_{23} = 3$, and $m_{24} = k-6$. Consequently,

$$TI_f(T^*) = kf(1,4) + 3f(2,3) + (k-6)f(2,4) + (n-2k+2)f(2,2).$$

Taking into account the above situations, the theorem is proven. □

5. Applications

In this section, we consider the VDB topological indices in Table 1. It is not difficult to verify that all VDB topological indices match the following lemma, and the detailed calculations are omitted herein.

Table 1. Some VDB topological indices.

No.	Indices	$f(x,y)$	Reference
1	Reciprocal sum-connectivity index	$\sqrt{x+y}$	[26]
2	Sombor index	$\sqrt{x^2+y^2}$	[11,23]
3	Reduced Sombor index	$\sqrt{(x-1)^2+(y-1)^2}$	
4	Third Sombor index	$\sqrt{2}\pi\frac{x^2+y^2}{x+y}$	
5	Fourth Sombor index	$\frac{\pi}{2}(\frac{x^2+y^2}{x+y})^2$	
6	Euler Sombor index	$\sqrt{x^2+y^2+xy}$	

Lemma 5.1. *The VDB topological indices in Table 1 match the following conditions:*
(i) $3(f(4,4)-f(3,4)) + f(2,4) - f(3,3) + f(1,2) - f(1,3) > 0$,
(ii) $4(f(4,4)-f(3,4)) + f(2,2) - f(2,3) + f(1,2) - f(1,3) > 0$*, and*
(iii) $g(x) = f(x,s) - f(x,r)$ *is strictly decreasing with respect to* x*, where* $1 \leq r < s \leq 4$*, and* $1 \leq x \leq 4$.

Consequently, based on Lemma 5.1 and Theorems 4.1 and 4.2, we deduce the following theorem immediately. It should be noted that the results concerning the reciprocal sum-connectivity index and the Sombor index have been presented in [26] and [11,23].

Theorem 5.1. *Let* $T \in \mathcal{CT}_{n,k}$ *with* $k \geq 3$ *and* $n \geq k+2$*. For all VDB topological indices in Table 1,*
(i) If $3 \leq k \leq 4$*, then*

$$TI_f(T) \leq (k-1)f(1,k) + f(1,2) + (n-k-2)f(2,2) + f(2,k),$$

the equality occurs if and only if $T \cong \mathcal{B}_{n,k}$.
(ii) If $k \geq 6$ *is even, then*

$$TI_f(T) \leq \begin{cases} kf(1,4) + (2n-3k+2)f(2,4) + (2k-n-3)f(4,4), & n \leq 2k-4, \\ kf(1,4) + (k-4)f(2,4) + (n-2k+3)f(2,2), & n \geq 2k-3, \end{cases}$$

the equality occurs if and only if $T \in \mathcal{CT}^1$.

(iii) If $k \geq 5$ *is odd, then*

$$TI_f(T) \leq \begin{cases} 2f(1,3)+3f(1,4)+f(3,4), & k=5, n=7,\\ 2f(1,3)+3f(1,4)+f(2,3)+f(2,4)+(n-8)f(2,2), & k=5, n\geq 8,\\ f(1,3)+6f(1,4)+(n-10)(f(2,3)+f(2,4))+(12-n)f(3,4), & k=7, n=10,11,\\ f(1,3)+6f(1,4)+2(f(2,3)+f(2,4))+(n-12)f(2,2), & k=7, n\geq 12,\\ 9f(1,4)+(n-13)(f(2,3)+f(2,4))+(16-n)f(3,4), & k=9, 13\leq n\leq 15,\\ 9f(1,4)+3(f(2,3)+f(2,4))+(n-16)f(2,2), & k=9, n\geq 16,\\ kf(1,4)+3f(3,4)+(2n-3k+1)f(2,4)+(2k-n-5)f(4,4), & \\ \qquad k\geq 11, 16\leq n\leq 2k-6, & \\ kf(1,4)+(n-2k+5)f(2,3)+(2k-n-2)f(3,4)+(n-k-4)f(2,4), & \\ \qquad k\geq 11, 2k-5\leq n\leq 2k-3, & \\ kf(1,4)+3f(2,3)+(k-6)f(2,4)+(n-2k+2)f(2,2), & \\ \qquad k\geq 11, n\geq 2k-2, & \end{cases}$$

the equality occurs if and only if $T \in \mathcal{CT}^2$.

6. Conclusions

Our current work is to investigate the extremal problems of various VDB indices for chemical trees by proposing a universal method. Based on the structure of chemical trees and by applying several transformations, sufficient conditions for the maximum VDB index of chemical trees with given pendant vertices have been identified. Additionally, it has been verified that six degree-based topological indices satisfy these sufficient conditions.

In Reference [24], the authors addressed the problem of calculating various topological indices using a universal (cutting) method and confirmed that this method was applicable to all Szeged-like topological indices. However, when comparing the topological indices applicable to [24] and those of this paper, these two sets (of indices) are completely distinct. In other words, the two methods apply respectively to distance-based and degree-based topological indices and cannot be generalized to each other. Thus, this paper serves as a parallel extension of Reference [24]. Therefore, exploring more and improved universal methods that apply to multiple classes of topological indices will be a key research topic for our future work.

Use of Generative-AI tools declaration

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

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Conflict of interest

The author declares no conflict of interest.

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