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Chemical Trees with Maximal VDB Topological Indices

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Abstract

A general vertex-degree-based (VDB) topological index of a graph G is defined as

$$\mathcal{T}_f = \mathcal{T}_f(G) = \sum_{uv \in E(G)} f(d_G(u), d_G(v)),$$

where $f(x, y) > 0$ is a symmetric real function with $x \geq 1$ and $y \geq 1$. Let $\mathcal{CT}_n$ be the set of all chemical trees of order n, and let $\hat{T}_f = \max\{\mathcal{T}_f(T) \mid T \in \mathcal{CT}_n\}$. A chemical tree $T \in \mathcal{CT}_n$ is an n-optimal $\mathcal{T}_f$ chemical tree if $\mathcal{T}_f(T) = \hat{T}_f$.

One important topic in chemical graph theory is the extremal value problem of VDB topological indices over $\mathcal{CT}_n$. In this work, we get the following results.

(1) We propose six conditions (C1)-(C6) for the symmetric real function $f(x, y)$. For a VDB topological index $\mathcal{T}_f$ satisfied the conditions (C1)-(C6), we obtained the necessary and sufficient conditions for $T \in \mathcal{CT}_n$ to be an n-optimal $\mathcal{T}_f$ chemical tree.

(2) For twenty-five VDB topological indices (as shown in Table 4.1 of Section 4), the n-optimal $\mathcal{T}_f$ chemical trees are characterized, and the maximum $\mathcal{T}_f$ values are determined, too.

1 Introduction

A general vertex-degree-based (VDB for short) topological index of a graph G is given by

$$\mathcal{T}_f = \mathcal{T}_f(G) = \sum_{uv \in E(G)} f(d_G(u), d_G(v)), \quad (1)$$

where $f(x, y) > 0$ is a symmetric real function with $x \geq 1$ and $y \geq 1$.

A tree T is a chemical tree (or molecular tree) if $d_T(v) \leq 4$ for $v \in V(T)$. Let $\mathcal{CT}_n$ be the set of all chemical trees of order n, and let $\hat{T}_f = \max\{\mathcal{T}_f(T) \mid T \in \mathcal{CT}_n\}$. A chemical tree $T \in \mathcal{CT}_n$ is an n-optimal $\mathcal{T}_f$ chemical tree if $\mathcal{T}_f(T) = \hat{T}_f$.

The problem of finding extremal values of a VDB topological index over $\mathcal{CT}_n$ has attracted considerable attention in the mathematical-chemistry literature. It is well known that the n-optimal $\mathcal{T}_f$ chemical trees of some VDB topological indices $\mathcal{T}_f$ have been determined, for example, the Randić index χ ($f(x, y) = \frac{1}{\sqrt{xy}}$) [1,2]; geometrical-arithmetic index $\mathcal{GA}$ ($f(x, y) = \frac{2\sqrt{xy}}{x+y}$) [3, 4]; arithmetic-geometric index $\mathcal{AG}$ ($f(x, y) = \frac{x+y}{2\sqrt{xy}}$) [3, 4]; Harmonic index $\mathcal{H}$ ($f(x, y) = \frac{2}{x+y}$) [5]; first Zagreb index $\mathcal{M}_1$ ($f(x, y) = x+y$) [6, 7]; second Zagreb index $\mathcal{M}_2$ ($f(x, y) = xy$) [6, 7]; forgotten index $\mathcal{F}$ ($f(x, y) = x^2+y^2$) [8]; symmetric division deg index $\mathcal{SDD}$ ($f(x, y) = \frac{x}{y}+\frac{y}{x}$) [9]; Sombor index $\mathcal{SO}$ ($f(x, y) = \sqrt{x^2 + y^2}$) [10, 11]; reduced Sombor index $\mathcal{SO}_{red}$ ($f(x, y) = \sqrt{(x-1)^2 + (y-1)^2}$) [10]; inverse sum indeg index $\mathcal{ISI}$ ($f(x, y) = \frac{xy}{x+y}$) [12]; and exponential first Zagreb index $e^{\mathcal{M}_1}$ ($f(x, y) = e^{x+y}$) [7].

In this paper, we study VDB topological indices over $\mathcal{CT}_n$. The main aim is to establish a general theorem that can capture the common properties necessary for the n-optimal $\mathcal{T}_f$ chemical trees of all VDB topological indices $\mathcal{T}_f$ satisfying certain conditions. We also apply our results to obtain the maximum values of some VDB topological indices over $\mathcal{CT}_n$.

In Section 2, we propose six conditions for the symmetric real function $f(x, y)$, and prove that for a VDB topological index $\mathcal{T}_f$ satisfied these conditions, if a chemical tree T is an n-optimal $\mathcal{T}_f$ chemical tree, then the number of 2-vertices and 3-vertices in T is at most one.

In Section 3, we obtain the necessary and sufficient conditions for a chemical tree to be an n-optimal $\mathcal{T}_f$ chemical tree when the VDB topological index $\mathcal{T}_f$ satisfied these conditions.

In Section 4, as an application of the main theorem in Section 3, for twenty-five VDB topological indices $\mathcal{T}_f$ (as shown in Table 4.1 of Section 4), we completely characterize the n-optimal $\mathcal{T}_f$ chemical trees, and the maximum $\mathcal{T}_f$ values are determined, too.

2 Lemmas

Let $f(x,y) > 0$ be a symmetric real function with $x \geq 1$ and $y \geq 1$. In this section, we will consider the VDB topological indices $\mathcal{T}_f$ satisfied the following conditions:

(C1) $\frac{\partial f(x,y)}{\partial x} > 0$ and $\frac{\partial^2 f(x,y)}{\partial x^2} \geq 0$ for $x > 1$ and $y \geq 1$;

(C2) $f(1,4) - f(2,2) \geq 0$;

(C3) $f(1,3) + f(3,4) - f(2,2) - f(2,4) \geq 0$;

(C4) $f(2,4) + f(3,4) - 2f(3,3) \geq 0$;

(C5) $f(2,2) + f(4,4) - f(1,3) - f(3,4) \geq 0$;

(C6) $f(1,2) + f(4,4) - f(1,3) - f(3,3) \geq 0$.

Lemma 2.1. *Let $f(x,y) > 0$ be a symmetric real function satisfied the condition (C1). Then for any fixed $y \geq 1$, we have*

(1) $f(1,y) + f(4,y) \geq f(2,y) + f(3,y)$;

(2) $f(1,y) + f(3,y) \geq 2f(2,y)$;

(3) $f(2,y) + f(4,y) \geq 2f(3,y)$.

Proof. By Mean Value Theorem, §

$$\begin{aligned} f(1,y) + f(4,y) - f(2,y) - f(3,y) &= f(4,y) - f(3,y) - (f(2,y) - f(1,y)) \\ &= f'_x(\theta_{11}, y) - f'_x(\theta_{12}, y) \geq 0, \\ f(1,y) + f(3,y) - 2f(2,y) &= f(3,y) - f(2,y) - (f(2,y) - f(1,y)) \\ &= f'_x(\theta_{21}, y) - f'_x(\theta_{22}, y) \geq 0, \\ f(2,y) + f(4,y) - 2f(3,y) &= f(4,y) - f(3,y) - (f(3,y) - f(2,y)) \\ &= f'_x(\theta_{31}, y) - f'_x(\theta_{32}, y) \geq 0, \end{aligned}$$

where $\theta_{11} \in (3,4)$, $\theta_{12} \in (1,2)$, $\theta_{21} \in (2,3)$, $\theta_{22} \in (1,2)$, $\theta_{31} \in (3,4)$, and $\theta_{32} \in (2,3)$. ■

Let T be a tree of order n. A vertex $v \in V(T)$ will be called k-vertex if $d_T(v) = k$, and a edge $uv \in E(T)$ will be called a (k,ℓ)-edge if $d_T(u) = k$ and $d_T(v) = \ell$. Let us denote by $n_k(T)$ the number of k-vertices of T, and $m_{k,\ell}(T)$ the number of (k,ℓ)-edges of T.

Lemma 2.2. *Let $n \geq 7$, $f(x,y) > 0$ be a symmetric real function satisfied the conditions (C1)-(C6), and let $T \in \mathcal{CT}_n$ be n-optimal $\mathcal{T}_f$. Then $m_{2,3}(T) = 0$.*

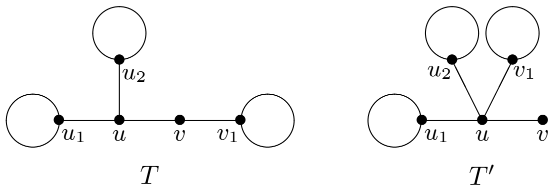

Figure 1. The chemical trees T and T' for Lemma 2.2.

Proof. Suppose to the contrary that $m_{2,3}(T) \geq 1$, that is, there is $uv \in E(T)$ such that $d_T(u) = 3$ and $d_T(v) = 2$. Let $N_T(u) = \{v, u_1, u_2\}$, $N_T(v) = \{u, v_1\}$, and $T' = T - vv_1 + uv_1$ (as depicted in Fig. 1). We claim that $\mathcal{T}_f(T') > \mathcal{T}_f(T)$.

Note that

$$\begin{aligned}\mathcal{T}_f(T') - \mathcal{T}_f(T) = {} & f(4, d_T(u_1)) + f(4, d_T(u_2)) + f(4, d_T(v_1)) + f(1,4) \\ & - f(3, d_T(u_1)) - f(3, d_T(u_2)) - f(2, d_T(v_1)) - f(2,3).\end{aligned}$$

Since $n \geq 7$, $\max\{d_T(u_1), d_T(u_2), d_T(v_1)\} \geq 2$. Without loss of generality, we assume that $d_T(u_1) \leq d_T(u_2)$.

Case 1. $2 \leq d_T(v_1) \leq 3$.

From the condition (C1), we deduce that $f(4, d_T(u_1)) > f(3, d_T(u_1))$, $f(4, d_T(u_2)) > f(3, d_T(u_2))$, $f(1,4) > f(1, d_T(v_1))$, and $f(3, d_T(v_1)) \geq f(2,3)$. By Lemma 2.1, we get $f(4, d_T(v_1)) + f(1, d_T(v_1)) \geq f(2, d_T(v_1)) +$

$f(3, d_T(v_1))$. Then

$$\begin{aligned}\mathcal{T}_f(T') - \mathcal{T}_f(T) &> f(4, d_T(v_1)) + f(1, d_T(v_1)) - f(2, d_T(v_1)) - f(2,3) \\ &\geq f(2, d_T(v_1)) + f(3, d_T(v_1)) - f(2, d_T(v_1)) - f(2,3) \geq 0.\end{aligned}$$

Case 2. $d_T(v_1) = 4$.

From the condition (C1), we deduce that $f(4, d_T(u_1)) > f(3, d_T(u_1))$ and $f(4, d_T(u_2)) > f(3, d_T(u_2))$. By Lemma 2.1, we get $f(4,4) + f(1,4) \geq f(2,4) + f(3,4) > f(2,4) + f(2,3)$. So

$$\mathcal{T}_f(T') - \mathcal{T}_f(T) > f(4,4) + f(1,4) - f(2,4) - f(2,3) > 0.$$

Case 3. $d_T(u_2) = 4$.

From the condition (C1), we deduce that $f(4, d_T(u_1)) > f(3, d_T(u_1))$ and $f(4, d_T(v_1)) > f(2, d_T(v_1))$. By Lemma 2.1, $f(4,4) + f(1,4) \geq f(2,4) + f(3,4) > f(2,3) + f(3,4)$. Then

$$\mathcal{T}_f(T') - \mathcal{T}_f(T) > f(4,4) + f(1,4) - f(3,4) - f(2,3) > 0.$$

Case 4. $d_T(v_1) = 1$ and $d_T(u_1) = d_T(u_2) = 3$.

From the conditions (C1), (C2) and (C4), we have $f(2,4) > f(2,3)$, $f(2,2) > f(1,2)$, $f(1,4) \geq f(2,2)$, and $f(3,4) \geq 2f(3,3) - f(2,4)$. By Lemma 2.1, $f(1,4) + f(3,4) \geq 2f(2,4)$. So

$$\begin{aligned}\mathcal{T}_f(T') - \mathcal{T}_f(T) = &(f(3,4) + f(1,4)) + f(3,4) + f(1,4) - 2f(3,3) \\ &- f(1,2) - f(2,3) \\ >&2f(2,4) + 2f(3,3) - f(2,4) + f(2,2) - 2f(3,3) \\ &- f(1,2) - f(2,3) \\ =&f(2,4) + f(2,2) - f(1,2) - f(2,3) > 0.\end{aligned}$$

Case 5. $d_T(v_1) = 1$ and $d_T(u_1) = 2$ (or $d_T(v_1) = 1$ and $d_T(u_2) = 2$).

From the conditions (C1) and (C2), we deduce that $f(4, d_T(u_2)) > f(3, d_T(u_2))$, and $f(1,4) \geq f(2,2) > f(1,2)$. By Lemma 2.1, we get

$f(2,4) + f(2,2) \geq 2f(2,3)$. Then

$$\mathcal{T}_f(T') - \mathcal{T}_f(T) > f(2,4) + 2f(1,4) - 2f(2,3) - f(1,2)$$
$$> f(2,4) + f(2,2) - 2f(2,3) \geq 0.$$

So $\mathcal{T}_f(T') > \mathcal{T}_f(T)$ and it contradicts that T is an n-optimal $\mathcal{T}_f$ chemical tree. ■

Lemma 2.3. *Let $n \geq 7$, $f(x,y) > 0$ be a symmetric real function satisfied the conditions (C1)-(C6), and $T \in \mathcal{CT}_n$ be n-optimal $\mathcal{T}_f$. Then $m_{2,2}(T) = 0$.*

Proof. Suppose to the contrary that $m_{2,2}(T) \geq 1$. We claim that there exists a chemical tree $T' \in \mathcal{CT}_n$ such that $\mathcal{T}_f(T') > \mathcal{T}_f(T)$.

Case 1. $n_4(T) = 0$.

By Lemma 2.2, $m_{2,3}(T) = 0$. Then $n_3(T) = 0$, and T is a path as depicted in Fig. 2. Let $T' = T - v_1v_2 - v_2v_3 - v_3v_4 - v_4v_5 + v_5v_1 + v_5v_2 + v_6v_3 + v_6v_4$.

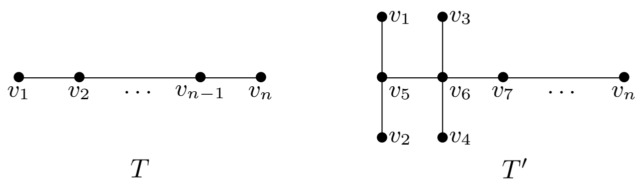

Figure 2. The chemical trees T and T' for Case 1 of Lemma 2.3.

If $n = 7$, then from the conditions (C1) and (C2), we have $f(1,3) > f(1,2)$, and $f(1,4) \geq f(2,2)$. By Lemma 2.1, $f(1,4) + f(3,4) \geq 2f(2,4) > 2f(2,2)$. So

$$\mathcal{T}_f(T') - \mathcal{T}_f(T) = 2f(1,3) + 3f(1,4) + f(3,4) - 2f(1,2) - 4f(2,2)$$
$$> 2f(1,3) + 2f(1,4) + 2f(2,2) - 2f(1,2) - 4f(2,2) > 0.$$

If $n \geq 8$, then from the conditions (C1) and (C2), we have $f(1,3) > f(1,2)$, $f(2,4) > f(2,2)$, and $f(1,4) \geq f(2,2)$. By Lemma 2.1, $f(1,3) +$

$f(3,4) = f(1,3) + f(4,3) \geq f(2,3) + f(3,3) > 2f(2,2)$. So

$$\begin{aligned}\mathcal{T}_f(T') - \mathcal{T}_f(T) &= 2f(1,3) + 2f(1,4) + f(3,4) + f(2,4) - f(1,2) - 5f(2,2)\\ &> f(1,3) + 2f(1,4) + 2f(2,2) + f(2,4) - f(1,2) - 5f(2,2)\\ &> 0.\end{aligned}$$

Case 2. $n_4(T) \geq 1$.

Let $uv \in E(T)$ be a $(2,2)$-edge, $N_T(u) = \{u_1, v\}$ and $N_T(v) = \{u, v_1\}$. By Lemma 2.2, $m_{2,3}(T) = 0$. Then we can choose the vertices u, v appropriately, such that $d_T(v_1) = 4$. Note that $d_T(u_1) \in \{1, 2, 4\}$.

Subcase 2.1. $d_T(u_1) = 2$.

Let $N_T(u_1) = \{u_2, u\}$, and $T' = T - uu_1 - u_1u_2 + vu_1 + vu_2$ as depicted in Fig. 3.

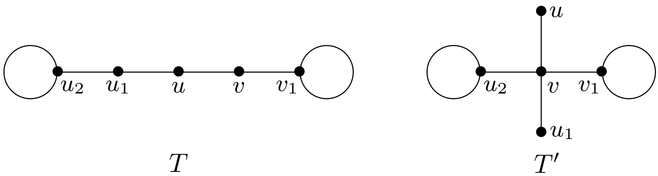

Figure 3. The chemical trees T and T' for Subcase 2.1 of Lemma 2.3.

From the condition (C1), we have $f(4, d_T(u_2)) > f(2, d_T(u_2))$. By Lemma 2.1, $f(4,4) + f(1,4) \geq f(2,4) + f(3,4)$, and $f(1,4) + f(3,4) \geq 2f(2,4) > 2f(2,2)$. Then

$$\begin{aligned}\mathcal{T}_f(T') - \mathcal{T}_f(T) =& f(4, d_T(u_2)) + f(4,4) + 2f(1,4) - f(2, d_T(u_2))\\ &- f(2,4) - 2f(2,2)\\ >& f(4,4) + 2f(1,4) - f(2,4) - 2f(2,2)\\ \geq& f(2,4) + f(3,4) + f(1,4) - f(2,4) - 2f(2,2) > 0.\end{aligned}$$

Subcase 2.2. $d_T(u_1) \neq 2$.

In this case $d_T(u_1) \in \{1, 4\}$. Let $T' = T - uu_1 + vu_1$ as depicted in Fig. 4.

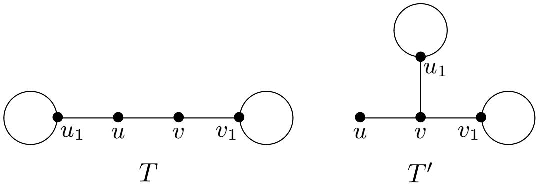

Figure 4. The chemical trees T and T' for Subcase 2.2 of Lemma 2.3.

If $d_T(u_1) = 1$, from the conditions (C1) and (C3), we get

$$\begin{aligned}\mathcal{T}_f(T') - \mathcal{T}_f(T) &= 2f(1,3) + f(3,4) - f(1,2) - f(2,2) - f(2,4)\\ &> f(1,3) + f(3,4) - f(2,2) - f(2,4) \geq 0.\end{aligned}$$

If $d_T(u_1) = 4$, from the conditions (C1) and (C3), we get

$$\begin{aligned}\mathcal{T}_f(T') - \mathcal{T}_f(T) &= f(1,3) + 2f(3,4) - f(2,2) - 2f(2,4)\\ &> f(1,3) + f(3,4) - f(2,2) - f(2,4) \geq 0.\end{aligned}$$

So $\mathcal{T}_f(T') > \mathcal{T}_f(T)$ and it contradicts that T is an n-optimal $\mathcal{T}_f$ chemical tree. ■

Lemma 2.4. *Let $n \geq 7$, $f(x,y) > 0$ be a symmetric real function satisfied the conditions (C1)-(C6), and $T \in \mathcal{CT}_n$ be n-optimal $\mathcal{T}_f$. Then $m_{3,3}(T) = 0$.*

Proof. Suppose to the contrary that $m_{3,3}(T) \geq 1$. We claim that there exists a chemical tree $T' \in \mathcal{CT}_n$ such that $\mathcal{T}_f(T') > \mathcal{T}_f(T)$.

Case 1. $n_4(T) = 0$.

By Lemma 2.2, $n_2(T) = 0$. Then the degrees of all vertices of T are from the set $\{1,3\}$. In this case, we can assume that T is a chemical tree as depicted in Fig. 5, where $d_T(v_1) = d_T(v_{m+1}) = 1$, $d_T(v_i) = 3$ and $d_T(u_i) \in \{1,3\}$ for $i = 2,3,\ldots,m$. Since $n \geq 7$, then $m \geq 4$.

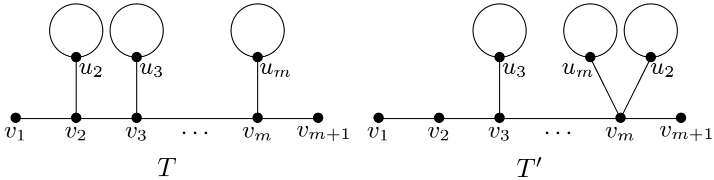

Figure 5. The chemical trees T and T' for Case 1 of Lemma 2.4.

Let $T' = T - v_2u_2 + v_mu_2$. Then

$$\begin{aligned}\mathcal{T}_f(T') - \mathcal{T}_f(T) =& f(4, d_T(u_2)) + f(4, d_T(u_m)) + f(1,4) + f(3,4) \\ &+ f(1,2) + f(3,2) - f(3, d_T(u_2)) - f(3, d_T(v_m)) \\ &- 2f(1,3) - 2f(3,3).\end{aligned}$$

From the condition (C1), we have $f(4, d_T(u_2)) > f(3, d_T(u_2))$ and $f(4, d_T(u_m)) > f(3, d_T(u_m))$. By Lemma 2.1, $f(1,4) + f(1,2) \geq 2f(1,3)$, and $f(3,4) + f(3,2) \geq 2f(3,3)$. Then $\mathcal{T}_f(T') > \mathcal{T}_f(T)$.

Case 2. $n_4(T) \geq 1$.

Let $uv \in E(T)$ be a $(3,3)$-edge, $N_T(u) = \{v, u_1, u_2\}$, and $N_T(v) = \{u, v_1, v_2\}$. By Lemma 2.2, the degrees of the vertices u_1, u_2, v_1, v_2 are from the set $\{1,3,4\}$. We can choose the vertices u, v appropriately, such that the set $\{u_1, u_2, v_1, v_2\}$ contains at least one 4-vertex. Without loss of generality, assume that $d_T(v_2) = 4$, and $d_T(u_1) \leq d_T(u_2)$. Let $T' = T - uu_2 + vu_2$ (see Fig. 6). Then

$$\begin{aligned}\mathcal{T}_f(T') - \mathcal{T}_f(T) =& f(2, d_T(u_1)) + f(4, d_T(u_2)) + f(4, d_T(v_1)) + f(2,4) \\ &+ f(4,4) - f(3, d_T(u_1)) - f(3, d_T(u_2)) - f(3, d_T(v_1)) \\ &- f(3,3) - f(3,4).\end{aligned}$$

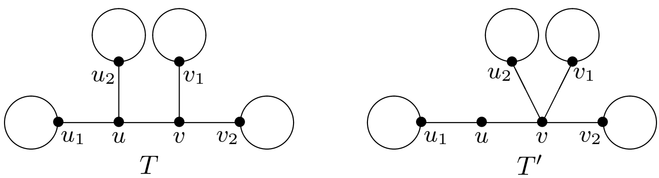

Figure 6. The chemical trees T and T' for Case 2 of Lemma 2.4.

From the condition (C1), we have $f(4, d_T(v_1)) > f(3, d_T(v_1))$. So

$$\begin{aligned}\mathcal{T}_f(T') - \mathcal{T}_f(T) > f(2, d_T(u_1)) + f(4, d_T(u_2)) + f(2,4) + f(4,4) \\ - f(3, d_T(u_1)) - f(3, d_T(u_2)) - f(3,3) - f(3,4).\end{aligned}$$

Kept in mind that the degrees of the vertices u_1, u_2 are from the set $\{1, 3, 4\}$, and $d_T(u_1) \le d_T(u_2)$.

Subcase 2.1. $d_T(u_1) = d_T(u_2) = 1$.

By Lemma 2.1, we have $f(1,2) + f(1,4) \ge 2f(1,3)$, and $f(2,4) + f(4,4) \ge 2f(3,4) > f(3,3) + f(3,4)$. Then

$$\begin{aligned}\mathcal{T}_f(T') - \mathcal{T}_f(T) >& f(1,2) + f(1,4) + f(2,4) + f(4,4) - 2f(1,3) \\ & - f(3,3) - f(3,4) > 0.\end{aligned}$$

Subcase 2.2. $d_T(u_1) = 1$ and $d_T(u_2) = 3$.

By Lemma 2.1, we have $f(1,2)+f(2,4) \ge f(2,2)+f(2,3)$, and $f(2,3)+f(3,4) \ge 2f(3,3)$. Then

$$\begin{aligned}\mathcal{T}_f(T') - \mathcal{T}_f(T) >& f(1,2) + f(3,4) + f(2,4) + f(4,4) - f(1,3) \\ & - 2f(3,3) - f(3,4) \\ \ge& f(2,2) + f(2,3) + f(3,4) + f(4,4) - f(1,3) \\ & - 2f(3,3) - f(3,4) \\ \ge& f(2,2) + 2f(3,3) + f(4,4) - f(1,3) - 2f(3,3) - f(3,4) \\ =& f(2,2) + f(4,4) - f(1,3) - f(3,4).\end{aligned}$$

From the condition (C5), $\mathcal{T}_f(T') > \mathcal{T}_f(T)$.

Subcase 2.3. $d_T(u_1) = 1$ and $d_T(u_2) = 4$.

By Lemma 2.1, we have $f(4,4) + f(2,4) \ge 2f(3,4)$. Then

$$\begin{aligned}\mathcal{T}_f(T') - \mathcal{T}_f(T) &> f(1,2) + 2f(4,4) + f(2,4) - f(1,3) - 2f(3,4) - f(3,3) \\ &\ge f(1,2) + f(4,4) + 2f(3,4) - f(1,3) - 2f(3,4) - f(3,3) \\ &= f(1,2) + f(4,4) - f(1,3) - f(3,3).\end{aligned}$$

From the condition (C6), $\mathcal{T}_f(T') > \mathcal{T}_f(T)$.

Subcase 2.4. $d_T(u_1) = 3$.

From the condition (C1), we have $f(4, d_T(u_2)) > f(3, d_T(u_2))$. By Lemma 2.1, $f(2,4) + f(4,4) \geq 2f(3,4)$, and $f(3,2) + f(3,4) \geq 2f(3,3)$. Then

$$\begin{aligned}\mathcal{T}_f(T') - \mathcal{T}_f(T) &> f(2,3) + f(2,4) + f(4,4) - 2f(3,3) - f(3,4) \\ &\geq f(2,3) + 2f(3,4) - 2f(3,3) - f(3,4) \\ &= f(2,3) + f(3,4) - 2f(3,3) \geq 0.\end{aligned}$$

Subcase 2.5. $d_T(u_1) = d_T(u_2) = 4$.

From the condition (C1), we have $f(3,4) > f(3,3)$. By Lemma 2.1, $f(2,4) + f(4,4) \geq 2f(3,4)$. Therefore

$$\begin{aligned}\mathcal{T}_f(T') - \mathcal{T}_f(T) &> 2f(2,4) + 2f(4,4) - 3f(3,4) - f(3,3) \\ &\geq 4f(3,4) - 3f(3,4) - f(3,3) > 0.\end{aligned}$$

So $\mathcal{T}_f(T') > \mathcal{T}_f(T)$ and it contradicts that T is an n-optimal $\mathcal{T}_f$ chemical tree. ■

By Lemmas 2.2-2.4, we have the following conclusion.

Theorem 2.5. *Let $n \geq 7$, $f(x,y) > 0$ be a symmetric real function satisfied the conditions (C1)-(C6), and $T \in \mathcal{CT}_n$ be n-optimal $\mathcal{T}_f$. Then $m_{2,3}(T) = 0$, $m_{2,2}(T) = 0$, and $m_{3,3}(T) = 0$.*

Lemma 2.6. *Let $f(x,y) > 0$ be a symmetric real function satisfied the conditions (C1)-(C6), and $T \in \mathcal{CT}_n$ be n-optimal $\mathcal{T}_f$. Then $n_2(T) \leq 1$.*

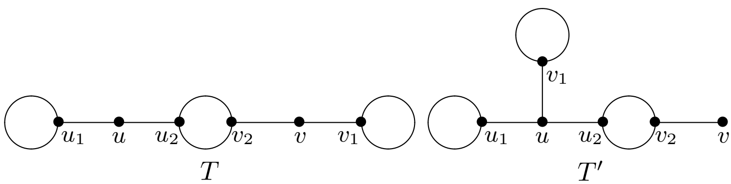

Figure 7. The chemical trees T and T' for Lemma 2.6.

Proof. Suppose to the contrary that $n_2(T) \geq 2$, that is, there are $u, v \in V(T)$ such that $d_T(u) = d_T(v) = 2$. By Theorem 2.5, $uv \notin E(T)$.

Let $N_T(u) = \{u_1, u_2\}$ and $N_T(v) = \{v_1, v_2\}$ such that the unique path from u to v goes through u_2 and v_2 as depicted in Fig. 7. By Theorem 2.5, $d_T(u_2) = d_T(v_2) = 4$.

Let $T' = T - vv_1 + uv_1$. From the condition (C1), we have $f(3, d_T(u_1)) > f(2, d_T(u_1))$, and $f(3, d_T(v_1)) > f(2, d_T(v_1))$. By Lemma 2.1, $f(1, 4) + f(3, 4) \geq 2f(2, 4)$. Then

$$\begin{aligned}\mathcal{T}_f(T') - \mathcal{T}_f(T) &= f(3, d_T(u_1)) + f(3, d_T(v_1)) + f(3, 4) + f(1, 4)\\ &\quad - f(2, d_T(u_1)) - f(2, d_T(v_1)) - 2f(2, 4) > 0,\end{aligned}$$

and it contradicts that T is an n-optimal $\mathcal{T}_f$ chemical tree. ■

Lemma 2.7. *Let $f(x, y) > 0$ be a symmetric real function satisfied the conditions (C1)-(C6), and $T \in \mathcal{CT}_n$ be n-optimal $\mathcal{T}_f$. Then $n_3(T) \leq 1$.*

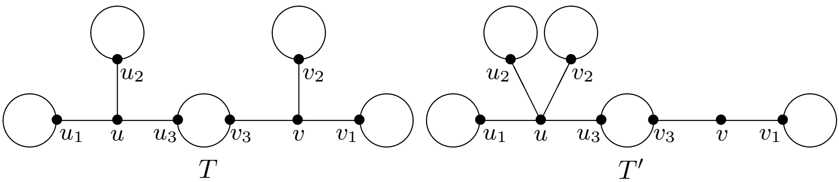

Figure 8. The chemical trees T and T' for Lemma 2.7.

Proof. Suppose to the contrary that $n_3(T) \geq 2$, that is, there are $u, v \in V(T)$ such that $d_T(u) = d_T(v) = 3$. By Theorem 2.5, $uv \notin E(T)$.

Let $N_T(u) = \{u_1, u_2, u_3\}$ and $N_T(v) = \{v_1, v_2, v_3\}$ such that the unique path from u to v goes through u_3 and v_3 as depicted in Fig. 8. By Theorem 2.5, $d_T(u_3) = d_T(v_3) = 4$, and the degrees of the vertices u_1, u_2, v_1, v_2 are from the set $\{1, 4\}$. Then at least two degrees of the vertices u_1, u_2, v_1, v_2 are the same. Without loss of generality, assume that $d_T(v_1) = d_T(u_1)$ (or $d_T(v_1) = d_T(v_2)$). Let $T' = T - vv_2 + uv_2$ (see Fig. 8).

From the condition (C1), we have $f(4, d_T(u_2)) > f(3, d_T(u_2))$, and $f(4, d_T(v_2)) > f(3, d_T(v_2))$. By Lemma 2.1, $f(2, 4) + f(4, 4) \geq 2f(3, 4)$.

Then

$$\begin{aligned}\mathcal{T}_f(T') - \mathcal{T}_f(T) =& f(4, d_T(u_1)) + f(4, d_T(u_2)) + f(4, d_T(v_2)) + f(4, 4) \\ &+ f(2, 4) + f(2, d_T(v_1)) - f(3, d_T(u_1)) - f(3, d_T(u_2)) \\ &- 2f(3, 4) - f(3, d_T(v_2)) - f(3, d_T(v_1)) \\ >& f(4, d_T(u_1)) + f(2, d_T(v_1)) - f(3, d_T(u_1)) - f(3, d_T(v_1)).\end{aligned}$$

Noting that $d_T(v_1) = d_T(u_1)$, by Lemma 2.1, $\mathcal{T}_f(T') - \mathcal{T}_f(T) > 0$. This result contradicts that T is an n-optimal $\mathcal{T}_f$ chemical tree. ■

Theorem 2.8. *Let $f(x, y) > 0$ be a symmetric real function satisfied the conditions (C1)-(C6), and $T \in \mathcal{CT}_n$ be n-optimal $\mathcal{T}_f$. Then $n_2(T) + n_3(T) \leq 1$.*

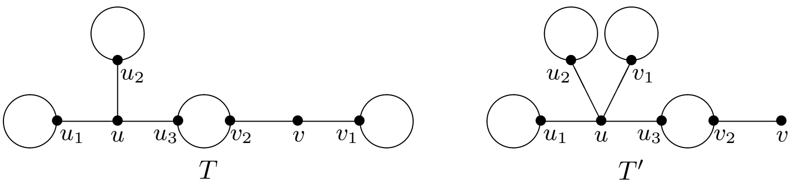

Figure 9. The chemical trees T and T' for Theorem 2.8.

Proof. By Lemmas 2.6 and 2.7, $n_2(T) + n_3(T) \leq 2$. Suppose to the contrary that $u, v \in V(T)$ with $d_T(u) = 3$, $d_T(v) = 2$, and u, v are not adjacent (due to Lemma 2.2). Let $N_T(u) = \{u_1, u_2, u_3\}$ and $N_T(v) = \{v_1, v_2\}$ such that unique path from u to v goes through u_3 and v_2 as depicted in Fig. 9. By Lemmas 2.6 and 2.7, $d_T(u_3) = d_T(v_2) = 4$. Let $T' = T - vv_1 + uv_1$. Then

$$\begin{aligned}\mathcal{T}_f(T') - \mathcal{T}_f(T) =& f(4, d_T(u_1)) + f(4, d_T(u_2)) + f(4, d_T(v_1)) + f(4, 4) \\ &+ f(1, 4) - f(3, d_T(u_1)) - f(3, d_T(u_2)) - f(3, 4) \\ &- f(2, 4) - f(2, d_T(v_1)) \\ >& f(4, 4) + f(1, 4) - f(3, 4) - f(2, 4).\end{aligned}$$

By Lemma 2.1, $\mathcal{T}_f(T') > \mathcal{T}_f(T)$, and it contradicts that T is an n-optimal $\mathcal{T}_f$ chemical tree. ■

3 Main Results

Let $f(x, y)$ satisfy the conditions (C1)-(C6). In this section, we will complete characterize the n-optimal $\mathcal{T}_f$ chemical trees. Denote

$$\mathcal{CT}_n^{(0)} = \{T \in \mathcal{CT}_n \mid n_2(T) = n_3(T) = 0\}, \tag{2}$$

$$\mathcal{CT}_n^{(1)} = \{T \in \mathcal{CT}_n \mid n_2(T) = 0, n_3(T) = 1, m_{1,3}(T) = 2, m_{3,4}(T) = 1\}, \tag{3}$$

$$\mathcal{CT}_n^{(2)} = \{T \in \mathcal{CT}_n \mid n_2(T) = 0, n_3(T) = 1, m_{1,3}(T) = 1, m_{3,4}(T) = 2\}, \tag{4}$$

$$\mathcal{CT}_n^{(3)} = \{T \in \mathcal{CT}_n \mid n_2(T) = 0, n_3(T) = 1, m_{1,3}(T) = 0, m_{3,4}(T) = 3\}, \tag{5}$$

$$\mathcal{CT}_n^{(4)} = \{T \in \mathcal{CT}_n \mid n_2(T) = 1, n_3(T) = 0, m_{1,2}(T) = 1, m_{2,4}(T) = 1\}, \tag{6}$$

$$\mathcal{CT}_n^{(5)} = \{T \in \mathcal{CT}_n \mid n_2(T) = 1, n_3(T) = 0, m_{1,2}(T) = 0, m_{2,4}(T) = 2\}. \tag{7}$$

Theorem 3.1. *Let $n \geq 7$, $f(x, y) > 0$ be a symmetric real function satisfied the conditions (C1)-(C6), and $T \in \mathcal{CT}_n$ be n-optimal $\mathcal{T}_f$. Then $T \in \bigcup_{i=0}^{i=5} \mathcal{CT}_n^{(i)}$.*

Proof. By Theorem 2.8, $n_2(T) + n_3(T) \leq 1$.

Case 1. $n_2(T) = n_3(T) = 0$. Then $T \in \mathcal{CT}_n^{(0)}$.

Case 2. $n_2(T) = 0$ and $n_3(T) = 1$.

Let u be the unique 3-vertex of T, and $N_T(u) = \{u_1, u_2, u_3\}$ with $d_T(u_1) \leq d_T(u_2) \leq d_T(u_3)$. Note that $n_2(T) = 0$. Then $d_T(u_i) \in \{1, 4\}$ for $i = 1, 2, 3$.

Subcase 2.1. If $d_T(u_1) = d_T(u_2) = 1$ and $d_T(u_3) = 4$, then $m_{1,3}(T) = 2$, and $m_{3,4}(T) = 1$, that is, $T \in \mathcal{CT}_n^{(1)}$.

Subcase 2.2. If $d_T(u_1) = 1$ and $d_T(u_3) = d_T(u_2) = 4$, then $m_{1,3}(T) = 1$, and $m_{3,4}(T) = 2$, that is, $T \in \mathcal{CT}_n^{(2)}$.

Subcase 2.3. If $d_T(u_1) = d_T(u_2) = d_T(u_3) = 4$, then $m_{1,3}(T) = 0$, and $m_{3,4}(T) = 3$, that is, $T \in \mathcal{CT}_n^{(3)}$.

So in this case, $T \in \mathcal{CT}_n^{(1)} \cup \mathcal{CT}_n^{(2)} \cup \mathcal{CT}_n^{(3)}$.

Case 3. $n_2(T) = 1$ and $n_3(T) = 0$.

Let v be the unique 2-vertex of T. Denote $N_T(v) = \{v_1, v_2\}$ with $d_T(v_1) \leq d_T(v_2)$. Then $d_T(v_i) \in \{1, 4\}$ for $i = 1, 2$.

Subcase 3.1. If $d_T(v_1) = 1$ and $d_T(v_2) = 4$, then $m_{1,2}(T) = 1$ and $m_{2,4}(T) = 1$, that is, $T \in \mathcal{CT}_n^{(4)}$;

Subcase 3.2. If $d_T(v_1) = d_T(v_2) = 4$, then $m_{1,2}(T) = 0$ and $m_{2,4}(T) = 2$, that is, $T \in \mathcal{CT}_n^{(5)}$.

So in this case, $T \in \mathcal{CT}_n^{(4)} \cup \mathcal{CT}_n^{(5)}$. ■

Note that for a chemical tree $T \in \mathcal{CT}_n$,

$$n_1(T) + n_2(T) + n_3(T) + n_4(T) = n, \tag{8}$$

$$n_1(T) + 2n_2(T) + 3n_3(T) + 4n_4(T) = 2(n-1), \tag{9}$$

$$m_{1,2}(T) + m_{1,3}(T) + m_{1,4}(T) = n_1(T), \tag{10}$$

$$m_{1,2}(T) + 2m_{2,2}(T) + m_{2,3}(T) + m_{2,4}(T) = 2n_2(T), \tag{11}$$

$$m_{1,3}(T) + m_{2,3}(T) + 2m_{3,3}(T) + m_{3,4}(T) = 3n_3(T), \tag{12}$$

$$m_{1,4}(T) + m_{2,4}(T) + m_{3,4}(T) + 2m_{4,4}(T) = 4n_4(T), \tag{13}$$

and

$$\mathcal{T}_f(T) = \sum_{uv \in E(T)} f(d_T(u), d_T(v)) = \sum_{1 \le k \le \ell \le 4} m_{k,\ell}(T) f(k, \ell). \tag{14}$$

Lemma 3.2. *Let $n \geq 7$ and $T \in \mathcal{CT}_n^{(0)}$. Then $n \equiv 2 (\mathrm{mod}\ 3)$, and*

$$\mathcal{T}_f(T) = \frac{2n+2}{3} f(1,4) + \frac{n-5}{3} f(4,4).$$

Proof. Note that $n_2(T) = n_3(T) = 0$. By (8) and (9),

$$n_1(T) + n_4(T) = n,$$
$$n_1(T) + 4n_4(T) = 2(n-1).$$

Then $n_1(T) = \frac{2n+2}{3}$, $n_4(T) = \frac{n-2}{3}$, and $n \equiv 2 (\mathrm{mod}\ 3)$. By (10) and (13), $m_{1,4}(T) = n_1(T) = \frac{2n+2}{3}$ and $m_{4,4}(T) = 2n_4(T) - \frac{1}{2} m_{1,4}(T) = \frac{n-5}{3}$, which combined with (14) yields

$$\begin{aligned}\mathcal{T}_f(T) &= m_{1,4}(T) f(1,4) + m_{4,4}(T) f(4,4) \\ &= \frac{2n+2}{3} f(1,4) + \frac{n-5}{3} f(4,4).\end{aligned}$$

■

Lemma 3.3. *Let $n \geq 7$ and $T \in \mathcal{CT}_n^{(1)} \cup \mathcal{CT}_n^{(2)} \cup \mathcal{CT}_n^{(3)}$.*

Then $n \equiv 1 (\text{mod } 3)$, *and*

$$\mathcal{T}_f(T) = \begin{cases} 2f(1,3) + f(3,4) + \frac{2n-5}{3} f(1,4) + \frac{n-7}{3} f(4,4), & \text{if } T \in \mathcal{CT}_n^{(1)}, \\ f(1,3) + 2f(3,4) + \frac{2n-2}{3} f(1,4) + \frac{n-10}{3} f(4,4), & \text{if } T \in \mathcal{CT}_n^{(2)}, \\ 3f(3,4) + \frac{2n+1}{3} f(1,4) + \frac{n-13}{3} f(4,4), & \text{if } T \in \mathcal{CT}_n^{(3)}. \end{cases}$$

Proof. Noticing that $n_2(T) = 0$ and $n_3(T) = 1$, by (8) and (9),

$$n_1(T) + n_4(T) + 1 = n,$$
$$n_1(T) + 3 + 4n_4(T) = 2(n-1).$$

Then $n_1(T) = \frac{2n+1}{3}$, $n_4(T) = \frac{n-4}{3}$, and $n \equiv 1 (\text{mod } 3)$. By (14),

$$\mathcal{T}_f(T) = m_{1,3}(T) f(1,3) + m_{3,4}(T) f(3,4) + m_{1,4}(T) f(1,4) + m_{4,4}(T) f(4,4).$$

Case 1. $T \in \mathcal{CT}_n^{(1)}$.

Noting that $m_{1,3}(T) = 2$ and $m_{3,4}(T) = 1$, by (10) and (13), we get $m_{1,4}(T) = n_1(T) - m_{1,3}(T) = \frac{2n-5}{3}$, and $m_{4,4}(T) = 2n_4(T) - \frac{1}{2}((m_{1,4}(T) + m_{3,4}(T)) = \frac{n-7}{3}$. Then

$$\mathcal{T}_f(T) = 2f(1,3) + f(3,4) + \frac{2n-5}{3} f(1,4) + \frac{n-7}{3} f(4,4).$$

Case 2. $T \in \mathcal{CT}_n^{(2)}$.

Noting that $m_{1,3}(T) = 1$ and $m_{3,4}(T) = 2$, by (10) and (13), we get $m_{1,4}(T) = n_1(T) - m_{1,3}(T) = \frac{2n-2}{3}$, and $m_{4,4}(T) = 2n_4(T) - \frac{1}{2}(m_{1,4}(T) + m_{3,4}(T)) = \frac{n-10}{3}$. Then

$$\mathcal{T}_f(T) = f(1,3) + 2f(3,4) + \frac{2n-2}{3} f(1,4) + \frac{n-10}{3} f(4,4).$$

Case 3. $T \in \mathcal{CT}_n^{(3)}$.

Noting that $m_{1,3}(T) = 0$ and $m_{3,4}(T) = 3$, by (10) and (13), we get $m_{1,4}(T) = n_1(T) = \frac{2n+1}{3}$, and $m_{4,4}(T) = 2n_4(T) - \frac{1}{2}\left(m_{1,4}(T) + m_{3,4}(T)\right) = \frac{n-13}{3}$. Then

$$\mathcal{T}_f(T) = 3f(3,4) + \frac{2n+1}{3} f(1,4) + \frac{n-13}{3} f(4,4).$$

■

Lemma 3.4. *Let $n \geq 7$ and $T \in \mathcal{CT}_n^{(4)} \cup \mathcal{CT}_n^{(5)}$. Then $n \equiv 0(\mathrm{mod}\ 3)$, and*

$$\mathcal{T}_f(T) = \begin{cases} f(1,2) + f(2,4) + \frac{2n-3}{3} f(1,4) + \frac{n-6}{3} f(4,4), & \text{if } T \in \mathcal{CT}_n^{(4)}, \\ 2f(2,4) + \frac{2n}{3} f(1,4) + \frac{n-9}{3} f(4,4), & \text{if } T \in \mathcal{CT}_n^{(5)}. \end{cases}$$

Proof. Noticing that $n_2(T) = 1$ and $n_3(T) = 0$, by (8) and (9),

$$n_1(T) + 1 + n_4(T) = n,$$
$$n_1(T) + 2 + 4n_4(T) = 2(n-1).$$

So $n_1(T) = \frac{2n}{3}$, $n_4(T) = \frac{n-3}{3}$, and $n \equiv 0(\mathrm{mod}\ 3)$. By (14),

$$\mathcal{T}_f(T) = m_{1,2}(T)f(1,2) + m_{2,4}(T)f(2,4) + m_{1,4}(T)f(1,4) + m_{4,4}(T)f(4,4).$$

Case 1. $T \in \mathcal{CT}_n^{(4)}$.

Noting that $m_{1,2}(T) = 1$ and $m_{2,4}(T) = 1$, by (10) and (13), we get $m_{1,4}(T) = n_1(T) - m_{1,2}(T) = \frac{2n-3}{3}$, and $m_{4,4}(T) = 2n_4(T) - \frac{1}{2}(m_{1,4}(T) + m_{2,4}(T)) = \frac{n-6}{3}$. Then

$$\mathcal{T}_f(T) = f(1,2) + f(2,4) + \frac{2n-3}{3} f(1,4) + \frac{n-6}{3} f(4,4).$$

Case 2. $T \in \mathcal{CT}_n^{(5)}$.

Noting that $m_{1,2}(T) = 0$ and $m_{2,4}(T) = 2$, by (10) and (13), we get $m_{1,4}(T) = n_1(T) = \frac{2n}{3}$, and $m_{4,4}(T) = 2n_4(T) - \frac{1}{2}\left(m_{1,4}(T) + m_{2,4}(T)\right) = \frac{n-9}{3}$. Then

$$\mathcal{T}_f(T) = 2f(2,4) + \frac{2n}{3} f(1,4) + \frac{n-9}{3} f(4,4).$$

■

By Lemmas 3.2, 3.3, and 3.4, we can use $\mathcal{T}_f^{(i)}$ to denote the VDB topological index $\mathcal{T}_f$ of the chemical trees in $\mathcal{CT}_n^{(i)}$ for $i = 0, 1, \ldots, 5$, that is,

$$\mathcal{T}_f^{(0)} = \frac{2n+2}{3} f(1,4) + \frac{n-5}{3} f(4,4), \tag{15}$$

$$\mathcal{T}_f^{(1)} = 2f(1,3) + f(3,4) + \frac{2n-5}{3} f(1,4) + \frac{n-7}{3} f(4,4), \tag{16}$$

$$\mathcal{T}_f^{(2)} = f(1,3) + 2f(3,4) + \frac{2n-2}{3} f(1,4) + \frac{n-10}{3} f(4,4), \tag{17}$$

$$\mathcal{T}_f^{(3)} = 3f(3,4) + \frac{2n+1}{3} f(1,4) + \frac{n-13}{3} f(4,4), \tag{18}$$

$$\mathcal{T}_f^{(4)} = f(1,2) + f(2,4) + \frac{2n-3}{3} f(1,4) + \frac{n-6}{3} f(4,4), \tag{19}$$

$$\mathcal{T}_f^{(5)} = 2f(2,4) + \frac{2n}{3} f(1,4) + \frac{n-9}{3} f(4,4). \tag{20}$$

Take

$$A_f = f(1,4) + f(3,4) - f(1,3) - f(4,4), \tag{21}$$

$$B_f = f(1,4) + f(2,4) - f(1,2) - f(4,4). \tag{22}$$

Then

$$\mathcal{T}_f^{(3)} - \mathcal{T}_f^{(2)} = \mathcal{T}_f^{(2)} - \mathcal{T}_f^{(1)} = A_f, \quad \mathcal{T}_f^{(5)} - \mathcal{T}_f^{(4)} = B_f. \tag{23}$$

So

$$\begin{cases} \mathcal{T}_f^{(1)} > \mathcal{T}_f^{(2)} > \mathcal{T}_f^{(3)}, & \text{if } A_f < 0, \\ \mathcal{T}_f^{(3)} > \mathcal{T}_f^{(2)} > \mathcal{T}_f^{(1)}, & \text{if } A_f > 0, \\ \mathcal{T}_f^{(1)} = \mathcal{T}_f^{(2)} = \mathcal{T}_f^{(3)}, & \text{if } A_f = 0, \end{cases} \tag{3.23}$$

and

$$\begin{cases} \mathcal{T}_f^{(4)} > \mathcal{T}_f^{(5)}, & \text{if } B_f < 0, \\ \mathcal{T}_f^{(5)} > \mathcal{T}_f^{(4)}, & \text{if } B_f > 0, \\ \mathcal{T}_f^{(4)} = \mathcal{T}_f^{(5)}, & \text{if } B_f = 0, \end{cases} \tag{3.24}$$

The following is the main theorem of this section.

Theorem 3.5. *Let $n \geq 7$, $f(x,y) > 0$ be a symmetric real function satisfied the conditions (C1)-(C6), and $T \in \mathcal{CT}_n$.*

(1) If $n \equiv 2 (\mathrm{mod}\ 3)$, then T is an n-optimal $\mathcal{T}_f$ chemical tree when and only when $T \in \mathcal{CT}_n^{(0)}$, and $\hat{T}_f = \mathcal{T}_f^{(0)}$.

(2) If $n \equiv 1 (\mathrm{mod}\ 3)$ *and* $A_f < 0$*, then* T *is an* n*-optimal* $\mathcal{T}_f$ *chemical tree when and only when* $T \in \mathcal{CT}_n^{(1)}$*, and* $\hat{T}_f = \mathcal{T}_f^{(1)}$*.*

If $n \equiv 1 (\mathrm{mod}\ 3)$ *and* $A_f > 0$*, then* T *is an* n*-optimal* $\mathcal{T}_f$ *chemical tree when and only when* $T \in \mathcal{CT}_n^{(3)}$*, and* $\hat{T}_f = \mathcal{T}_f^{(3)}$*.*

If $n \equiv 1 (\mathrm{mod}\ 3)$ *and* $A_f = 0$*, then* T *is an* n*-optimal* $\mathcal{T}_f$ *chemical tree when and only when* $T \in \mathcal{CT}_n^{(1)} \cup \mathcal{CT}_n^{(2)} \cup \mathcal{CT}_n^{(3)}$*, and* $\hat{T}_f = \mathcal{T}_f^{(1)} = \mathcal{T}_f^{(2)} = \mathcal{T}_f^{(3)}$*.*

(3) If $n \equiv 0 (\mathrm{mod}\ 3)$ *and* $B_f < 0$*, then* T *is an* n*-optimal* $\mathcal{T}_f$ *chemical tree when and only when* $T \in \mathcal{CT}_n^{(4)}$*, and* $\hat{T}_f = \mathcal{T}_f^{(4)}$*.*

If $n \equiv 0 (\mathrm{mod}\ 3)$ *and* $B_f > 0$*, then* T *is an* n*-optimal* $\mathcal{T}_f$ *chemical tree when and only when* $T \in \mathcal{CT}_n^{(5)}$*, and* $\hat{T}_f = \mathcal{T}_f^{(5)}$*.*

If $n \equiv 0 (\mathrm{mod}\ 3)$ *and* $B_f = 0$*, then* T *is an* n*-optimal* $\mathcal{T}_f$ *chemical tree when and only when* $T \in \mathcal{CT}_n^{(4)} \cup \mathcal{CT}_n^{(5)}$*, and* $\hat{T}_f = \mathcal{T}_f^{(4)} = \mathcal{T}_f^{(5)}$*.*

Proof. **Case 1.** $n \equiv 2 (\mathrm{mod}\ 3)$.

By Lemmas 3.2, 3.3 and 3.4, $\mathcal{CT}_n^{(0)} \neq \phi$, and $\mathcal{CT}_n^{(i)} = \phi$ for $i = 1, \ldots, 5$. So $\bigcup_{i=0}^{i=5} \mathcal{CT}_n^{(i)} = \mathcal{CT}_n^{(0)}$. By Theorem 3.1, T is an n-optimal $\mathcal{T}_f$ chemical tree when and only when $T \in \mathcal{CT}_n^{(0)}$. The maximum index value $\hat{T}_f = \mathcal{T}_f^{(0)}$.

Case 2. $n \equiv 1 (\mathrm{mod}\ 3)$.

By Lemmas 3.2, 3.3 and 3.4, $\mathcal{CT}_n^{(1)} \cup \mathcal{CT}_n^{(2)} \cup \mathcal{CT}_n^{(3)} \neq \phi$, and $\mathcal{CT}_n^{(i)} = \phi$ for $i = 0, 4, 5$. So $\bigcup_{i=0}^{i=5} \mathcal{CT}_n^{(i)} = \mathcal{CT}_n^{(1)} \cup \mathcal{CT}_n^{(2)} \cup \mathcal{CT}_n^{(3)}$. By Theorem 3.1 and Eq. (3.23), we have

- If $A_f < 0$, then T is an n-optimal $\mathcal{T}_f$ chemical tree when and only when $T \in \mathcal{CT}_n^{(1)}$, and $\hat{T}_f = \mathcal{T}_f^{(1)}$.
- If $A_f > 0$, then T is an n-optimal $\mathcal{T}_f$ chemical tree when and only when $T \in \mathcal{CT}_n^{(3)}$, and $\hat{T}_f = \mathcal{T}_f^{(3)}$.
- If $A_f = 0$, then T is an n-optimal $\mathcal{T}_f$ chemical tree when and only when $T \in \mathcal{CT}_n^{(1)} \cup \mathcal{CT}_n^{(2)} \cup \mathcal{CT}_n^{(3)}$, and $\hat{T}_f = \mathcal{T}_f^{(1)} = \mathcal{T}_f^{(2)} = \mathcal{T}_f^{(3)}$.

Case 3. $n \equiv 0 (\mathrm{mod}\ 3)$.

By Lemmas 3.2, 3.3 and 3.4, $\mathcal{CT}_n^{(4)} \cup \mathcal{CT}_n^{(5)} \neq \phi$ and $\mathcal{CT}_n^{(i)} = \phi$ for $i = 0, 1, 2, 3$, and so $\bigcup_{i=0}^{i=5} \mathcal{CT}_n^{(i)} = \mathcal{CT}_n^{(4)} \cup \mathcal{CT}_n^{(5)}$. By Theorem 3.1 and Eq. (3.24), we have

- If $B_f < 0$, then T is an n-optimal $\mathcal{T}_f$ chemical tree when and only when $T \in \mathcal{CT}_n^{(4)}$, and $\hat{T}_f = \mathcal{T}_f^{(4)}$.

- If $B_f > 0$, then T is an n-optimal $\mathcal{T}_f$ chemical tree when and only when $T \in \mathcal{CT}_n^{(5)}$, and $\hat{T}_f = \mathcal{T}_f^{(5)}$.

- If $B_f = 0$, then T is an n-optimal $\mathcal{T}_f$ chemical tree when and only when $T \in \mathcal{CT}_n^{(4)} \cup \mathcal{CT}_n^{(5)}$, and $\hat{T}_f = \mathcal{T}_f^{(4)} = \mathcal{T}_f^{(5)}$.

The theorem now follows. ■

4 Applications

In this section, we will consider the following twenty-five VDB topological indices (as shown in Table 4.1), and characterize the n-optimal $\mathcal{T}_f$ chemical trees.

Table 4.1 Some VDB topological indices $\mathcal{T}_f$

No.	Name	$f(x,y)$	A_f	B_f	Ref.
1	Sombor index	$\sqrt{x^2+y^2}$	$\mathcal{SO}$	$A_f > 0$, $B_f > 0$	[10, 11]
2	Reduced Sombor index	$\sqrt{(x-1)^2+(y-1)^2}$	$\mathcal{SO}_{red}$	$A_f > 0$, $B_f > 0$	[10, 11]
3	First Zagreb index	$x+y$	$\mathcal{M}_1$	$A_f = 0$, $B_f = 0$	[6, 7]
4	Forgotten index	x^2+y^2	$\mathcal{F}$	$A_f = 0$, $B_f = 0$	[8]
5	Second Zagreb index	xy	$\mathcal{M}_2$	$A_f < 0$, $B_f < 0$	[6, 7]
6	First hyper-Zagreb index	$(x+y)^2$	$\mathcal{HM}_1$	$A_f < 0$, $B_f < 0$	
7	Second hyper-Zagreb index	$(xy)^2$	$\mathcal{HM}_2$	$A_f < 0$, $B_f < 0$	
8	First Gourava index	$x+y+xy$	$\mathcal{GO}_1$	$A_f < 0$, $B_f < 0$	
9	Second Gourava index	$(x+y)xy$	$\mathcal{GO}_2$	$A_f < 0$, $B_f < 0$	
10	First hyper-Gourava index	$(x+y+xy)^2$	$\mathcal{HGO}_1$	$A_f < 0$, $B_f < 0$	
11	Second hyper-Gourava index	$((x+y)xy)^2$	$\mathcal{HGO}_2$	$A_f < 0$, $B_f < 0$	
12	Exponential Sombor index	$e^{\sqrt{x^2+y^2}}$	$e^{\mathcal{SO}}$	$A_f < 0$, $B_f < 0$	

13	Exponential reduced Sombor index	$e^{\sqrt{(x-1)^2+(y-1)^2}}$	$e^{\mathcal{SO}_{red}}$	$A_f < 0$, $B_f < 0$	
14	Exponential first Zagreb index	e^{x+y}	$e^{\mathcal{M}_1}$	$A_f < 0$, $B_f < 0$	[7]
15	Exponential forgotten index	$e^{x^2+y^2}$	$e^{\mathcal{F}}$	$A_f < 0$, $B_f < 0$	
16	Exponential second Zagreb index	e^{xy}	$e^{\mathcal{M}_2}$	$A_f < 0$, $B_f < 0$	
17	Exponential reciprocal Randić index	$e^{\sqrt{xy}}$	$e^{\mathcal{RR}}$	$A_f < 0$, $B_f < 0$	
18	Exponential reciprocal sum-connectivity index	$e^{\sqrt{x+y}}$	$e^{\mathcal{RSC}}$	$A_f < 0$, $B_f < 0$	
19	Exponential first hyper-Zagreb index	$e^{(x+y)^2}$	$e^{\mathcal{HM}_1}$	$A_f < 0$, $B_f < 0$	
20	Exponential second hyper-Zagreb index	$e^{(xy)^2}$	$e^{\mathcal{HM}_2}$	$A_f < 0$, $B_f < 0$	
21	Exponential first Gourava index	e^{x+y+xy}	$e^{\mathcal{GO}_1}$	$A_f < 0$, $B_f < 0$	
22	Exponential second Gourava index	$e^{(x+y)xy}$	$e^{\mathcal{GO}_2}$	$A_f < 0$, $B_f < 0$	
23	Exponential first hyper-Gourava index	$e^{(x+y+xy)^2}$	$e^{\mathcal{HGO}_1}$	$A_f < 0$, $B_f < 0$	
24	Exponential second hyper-Gourava index	$e^{((x+y)xy)^2}$	$e^{\mathcal{HGO}_2}$	$A_f < 0$, $B_f < 0$	
25	Exponential product-connectivity Gourava index	$e^{\sqrt{(x+y)xy}}$	$e^{\mathcal{PCG}}$	$A_f < 0$, $B_f < 0$	

It is not difficult to verify that these VDB topological indices satisfy the conditions (C1)-(C6). By Theorem 3.5, the following three theorems are straightforward.

Theorem 4.1. *Let $n \geq 7$ and $T \in \mathcal{CT}_n$. Then for the Sombor index and reduced Sombor index, the following results hold.*

(1) If $n \equiv 2 \pmod 3$, then T is an n-optimal $\mathcal{T}_f$ chemical tree when and only when $T \in \mathcal{CT}_n^{(0)}$, and

$$\hat{T}_f = \frac{2n+2}{3} f(1,4) + \frac{n-5}{3} f(4,4).$$

(2) If $n \equiv 1 \pmod 3$, then T is an n-optimal $\mathcal{T}_f$ chemical tree when and only when $T \in \mathcal{CT}_n^{(3)}$, and

$$\hat{T}_f = 3f(3,4) + \frac{2n+1}{3} f(1,4) + \frac{n-13}{3} f(4,4).$$

(3) If $n \equiv 0 (\mathrm{mod}\ 3)$*, then* T *is an* n*-optimal* $\mathcal{T}_f$ *chemical tree when and only when* $T \in \mathcal{CT}_n^{(5)}$*, and*

$$\hat{T}_f = 2f(2,4) + \frac{2n}{3} f(1,4) + \frac{n-9}{3} f(4,4).$$

Theorem 4.2. *Let* $n \geq 7$ *and* $T \in \mathcal{CT}_n$*. Then for the first Zagreb index and forgotten index, the following results hold.*

(1) If $n \equiv 2 (\mathrm{mod}\ 3)$*, then* T *is an* n*-optimal* $\mathcal{T}_f$ *chemical tree when and only when* $T \in \mathcal{CT}_n^{(0)}$*, and*

$$\hat{T}_f = \frac{2n+2}{3} f(1,4) + \frac{n-5}{3} f(4,4).$$

(2) If $n \equiv 1 (\mathrm{mod}\ 3)$*, then* T *is an* n*-optimal* $\mathcal{T}_f$ *chemical tree when and only when* $T \in \mathcal{CT}_n^{(1)} \cup \mathcal{CT}_n^{(2)} \cup \mathcal{CT}_n^{(3)}$*, and*

$$\hat{T}_f = 2f(1,3) + f(3,4) + \frac{2n-5}{3} f(1,4) + \frac{n-7}{3} f(4,4).$$

(3) If $n \equiv 0 (\mathrm{mod}\ 3)$*, then* T *is an* n*-optimal* $\mathcal{T}_f$ *chemical tree when and only when* $T \in \mathcal{CT}_n^{(4)} \cup \mathcal{CT}_n^{(5)}$*, and*

$$\hat{T}_f = f(1,2) + f(2,4) + \frac{2n-3}{3} f(1,4) + \frac{n-6}{3} f(4,4).$$

Theorem 4.3. *Let* $n \geq 7$ *and* $T \in \mathcal{CT}_n$*. Then for the VDB topological indices numbered from* 5 *to* 25 *as shown in Table 4.1, the following results hold.*

(1) If $n \equiv 2 (\mathrm{mod}\ 3)$*, then* T *is an* n*-optimal* $\mathcal{T}_f$ *chemical tree when and only when* $T \in \mathcal{CT}_n^{(0)}$*, and*

$$\hat{T}_f = \frac{2n+2}{3} f(1,4) + \frac{n-5}{3} f(4,4).$$

(2) If $n \equiv 1 (\mathrm{mod}\ 3)$*, then* T *is an* n*-optimal* $\mathcal{T}_f$ *chemical tree when and only when* $T \in \mathcal{CT}_n^{(1)}$*, and*

$$\hat{T}_f = 2f(1,3) + f(3,4) + \frac{2n-5}{3} f(1,4) + \frac{n-7}{3} f(4,4).$$

(3) If $n \equiv 0 (\bmod 3)$*, then* T *is an* n*-optimal* $\mathcal{T}_f$ *chemical tree when and only when* $T \in \mathcal{CT}_n^{(4)}$*, and*

$$\hat{T}_f = f(1,2) + f(2,4) + \frac{2n-3}{3} f(1,4) + \frac{n-6}{3} f(4,4).$$

In particularly, for the exponential reduced Sombor index $e^{\mathcal{SO}_{red}}$, induced by $f(x,y) = e^{\sqrt{(x-1)^2+(y-1)^2}}$, we have the following result. This result shows that Conjecture 3.1 in [13] is incorrect.

Corollary 4.4. *Let* $n \geq 7$ *and* $T \in \mathcal{CT}_n$*. Then for the exponential reduced Sombor index, the following results hold.*

(1) If $n \equiv 2 (\bmod 3)$*, then* T *is an* n*-optimal* $\mathcal{T}_f$ *chemical tree when and only when* $T \in \mathcal{CT}_n^{(0)}$*. The maximal exponential reduced Sombor index is*

$$\frac{1}{3}(n-5)e^{3\sqrt{2}} + \frac{2}{3}(n+1)e^3.$$

(2) If $n \equiv 1 (\bmod 3)$*, then* T *is an* n*-optimal* $\mathcal{T}_f$ *chemical tree when and only when* $T \in \mathcal{CT}_n^{(1)}$*. The maximal exponential reduced Sombor index is*

$$\frac{1}{3}(n-7)e^{3\sqrt{2}} + \frac{1}{3}(2n-5)e^3 + e^{\sqrt{13}} + 2e^2.$$

(3) If $n \equiv 0 (\bmod 3)$*, then* T *is an* n*-optimal* $\mathcal{T}_f$ *chemical tree when and only when* $T \in \mathcal{CT}_n^{(4)}$*. The maximal exponential reduced Sombor index is*

$$\frac{1}{3}(2n-3)e^3 + \frac{1}{3}(n-6)e^{3\sqrt{2}} + e^{\sqrt{10}} + e.$$

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