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On the Minimum Vertex-Degree-Based Topological Indices of Trees with Given Pendent Vertices

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Abstract

A general VDB topological index of a tree T is defined as

$$TI_f(T) = \sum_{uv \in E(T)} f(d(u), d(v)),$$

where $f(x, y)$ is a real symmetric function for $x, y \geq 1$. This paper aims to solve the minimum value problems of VDB indices for trees with given pendent vertices through a unified approach. We present the sufficient conditions for achieving the minimum value and characterize the extremal graphs. As an application, we demonstrate that fifteen types of VDB indices satisfy these sufficient conditions.

1 Introduction

Let $G = (V(G), E(G))$ be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. If G contains no cycles, it is called a *tree*, denoted

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by T. A *chemical tree*, denoted by CT, is a tree with $d(v) \leq 4$ for all $v \in V(T)$, where $d(v)$ stands for the degree of vertex v. A vertex v is a *pendent vertex* or *a leaf* if $d(v) = 1$. Let us use $\mathcal{T}_{n,k}$ ($\mathcal{CT}_{n,k}$) to denote the set of trees (chemical trees) of order n and with k pendent vertices, and $\mathcal{T}_n$ represents the set of trees with order n. Other undefined definitions and terms can be referred to in Bondy's Graph Theory [3].

Topological indices of graphs are among the useful tools for characterizing the physical or chemical properties of molecules. They are employed to indicate and predict the physicochemical properties, biological activities, and other attributes of compounds [20]. Consequently, a large number of topological indices have been proposed and investigated [1,22], particularly the vertex-degree-based (VDB) topological indices [6, 17, 21].

A general VDB topological index of G is defined as follows

$$TI_f = TI_f(G) = \sum_{uv \in E(G)} f(d(u), d(v)),$$

where $f(x, y)$ is a real symmetric function for $x \geq 1$ and $y \geq 1$. Let $m_{x,y}$ be the number of edges in G with $(d(u), d(v)) = (x, y)$, and Δ represents the maximum degree. Then

$$TI_f = TI_f(G) = \sum_{1 \leq x \leq y \leq \Delta} m_{x,y} f(x, y). \tag{1}$$

Owing to the significance of (chemical) trees in chemical molecular structures, the problem of extremal values of the VDB topological index on trees remains one of the most extensively studied topics. Taking the Sombor index as an example, research on its related trees has been attracting growing attention. Gutman [8] investigated the extremum of the Sombor index for any tree T and connected graphs. Liu et al. [11] determined the maximum value of the Sombor index for chemical trees with even vertices $n \geq 6$. In 2023, Maitreyi et al. [15] determined the minimum Sombor index for trees of $n \geq 7$ with p pendent vertices. Later, they [16] partially identified the general Sombor indices of trees on the maximum and minimum values with given the number of pendent vertices. Recently, Ahmad and Das [2] have completely characterized the chemical trees with given pendants that maximize the general Sombor index. For more results on other indices for trees and chemical trees, refer to references [4, 7, 12].

Using a universal method to investigate the properties or extremum of topological indices is an important issue that scholars have been exploring for a long time. In 2005, Li and Zheng [13] introduced two transformations to uniformly investigate the maximum and minimum problems of some topological indices for trees. Tomescu [18, 19] utilized the properties of convex functions to study the extremal problems of several topological indices under different given conditions, as well as the properties of connected graphs. In 2022, based on the properties of convex functions, Hu et al. [9] determined the lower bounds of connected graphs on the vertex-degree function-index. Meanwhile, by examining different conditions satisfied by vertex-degree functions, the authors [10] derived the upper and lower bounds of the value of $TI_f(G)$. Furthermore, Li and Peng [14] presented a survey on investigating extremal problems and spectral problems about finding unified ways.

Very recently, by analyzing the structure of chemical trees and calculating the values of m_{ij} (where $i, j \leq 4$), Du and Sun [5] provided some extremal results on bond incident degree indices of chemical trees with a fixed order and a fixed number of leaves.

Inspired by [13] and [5], we continue our efforts to investigate the extremal problems of various VDB indices on trees via a unified approach. In Section 2, we present a new mathematical formula for $TI_f(T)$. Based on this formula, in Section 3, we derive the sufficient conditions for the minimum value of the VDB index of trees with given pendent vertices and characterize the relevant extremal graphs. As an application, we demonstrate that fifteen types of VDB indices, including the Euler Sombor index, the modified first Zagreb index, and the exponential reciprocal sum-connectivity index, satisfy these sufficient conditions.

2 Preliminaries

Since a tree T is trivial when it has only one or two vertices, throughout this paper, we assume that T is a tree with $n \geq 3$ vertices. Recall that

$m_{x,y}$ be the number of edges in T with $(d(u), d(v)) = (x, y)$, and we use n_x denotes the number of vertices with $d(u) = x$. Then, for any tree T, the following equations hold:

$$\begin{cases} \sum_{x=1}^{\Delta} n_x = n, \\ \sum_{x=1}^{\Delta} x \cdot n_x = 2n - 2, \\ \sum_{y=1,\neq x}^{\Delta} m_{xy} + 2m_{xx} = x \cdot n_x, \ \textit{where } 1 \leq x \leq \Delta. \end{cases} \tag{2}$$

For convenience, let $A_1 = \{(1, y) \in \mathbb{N} \times \mathbb{N} : 2 \leq y \leq n-1\}$, $A_2 = \{(x, y) \in \mathbb{N} \times \mathbb{N} : 2 \leq x \leq y \leq n-1 \textit{ and } x + y \leq n\} - \{(2,2), (2,3), (3,3)\}$, $A^* = A_1 \cup A_2$, and $A = A^* \cup \{(2,2), (2,3), (3,3)\}$. Let

$$g(x, y) = f(x, y) + f(3,3) - 2f(2,3) + 6(\frac{x+y}{xy} - 1)\big(f(3,3) - f(2,3)\big). \tag{3}$$

Clearly, $g(2,3) = g(3,3) = 0$.

Lemma 1. *Let T be a tree with n vertices. Then*

$$TI_f(T) = (2n+4)f(2,3) - (n+5)f(3,3) + g(2,2)m_{2,2} + \sum_{(x,y) \in A^*} g(x,y) m_{x,y}, \tag{4}$$

where $g(x, y)$ is defined in (3).

Proof. For $T \in \mathcal{T}_n$, the following relations are valid

$$\sum_{(x,y)\in A} \frac{x+y}{xy} m_{x,y} = n, \qquad \sum_{(x,y)\in A} m_{x,y} = n - 1.$$

The previous two expressions can be rewritten as

$$5m_{2,3} + 4m_{3,3} = 6n - 6m_{2,2} - 6 \sum_{(x,y)\in A^*} \frac{x+y}{xy} m_{x,y},$$

$$m_{2,3} + m_{3,3} = n - 1 - m_{2,2} - \sum_{(x,y)\in A^*} m_{x,y},$$

where $A^* = A_1 \cup A_2$. The solutions to the foregoing equations are

$$m_{2,3} = 2(n+2) - 2m_{2,2} + \sum_{(x,y)\in A^*} (4 - 6\frac{x+y}{xy})m_{x,y},$$

$$m_{3,3} = -5 - n + m_{2,2} - \sum_{(x,y)\in A^*} (5 - 6\frac{x+y}{xy})m_{x,y}.$$

Thus, according to Equation (1), we deduce that

$$\begin{aligned}
& TI_f(T) \\
&= f(2,3)m_{2,3} + f(3,3)m_{3,3} + f(2,2)m_{2,2} + \sum_{(x,y)\in A^*} f(x,y)m_{x,y} \\
&= f(2,3)\Big(2(n+2) - 2m_{2,2} + \sum_{(x,y)\in A^*} (4 - 6\frac{x+y}{xy})m_{x,y}\Big) \\
&+ f(3,3)\Big(- 5 - n + m_{2,2} - \sum_{(x,y)\in A^*} (5 - 6\frac{x+y}{xy})m_{x,y}\Big) + f(2,2)m_{2,2} \\
&+ \sum_{(x,y)\in A^*} g(x,y)m_{x,y} \\
&= (2n+4)f(2,3) - (n+5)f(3,3) + \Big(f(2,2) + f(3,3) - 2f(2,3)\Big)m_{2,2} \\
&+ \sum_{(x,y)\in A^*} (f(x,y) + f(3,3) - 2f(2,3) \\
&+ 6(\frac{x+y}{xy} - 1)(f(3,3) - f(2,3)))m_{x,y} \\
&= (2n+4)f(2,3) - (n+5)f(3,3) + g(2,2)m_{2,2} + \sum_{(x,y)\in A^*} g(x,y)m_{x,y}.
\end{aligned}$$

This completes the proof. ■

Lemma 2. *Let $T \in \mathcal{T}_{n,k}$ (where $k \geq 3$). If the edge counts in T satisfy $m_{1,2} = k$, $m_{2,2} \geq 0$, $m_{2,3} \geq 0$, $m_{3,3} \geq 0$, and $m_{x,y} = 0$ for all other (x,y) pairs, then T has the degree sequence $\pi(T) = (\underbrace{3,\cdots,3}_{k-2}, \underbrace{2,\cdots,2}_{n-2k+2}, \underbrace{1,\cdots,1}_{k})$. Furthermore, we have $k \leq m_{2,3} \leq 3k-6$.*

Proof. Clearly, $n_1 = m_{1,2} = k$. From the conditions of the lemma, we obtain $n_i = 0$ for all $i \geq 4$. Moreover, according to Equation (2), we can derive that

$$n_1 + n_2 + n_3 = n,\ n_1 + 2n_2 + 3n_3 = 2n - 2.$$

Hence, $n_1 = k$, $n_2 = n - 2k + 2$, $n_3 = k - 2$. Therefore, T has the degree sequence

$$\pi(T) = (\underbrace{3, \cdots, 3}_{k-2}, \underbrace{2, \cdots, 2}_{n-2k+2}, \underbrace{1, \cdots, 1}_{k}).$$

We now prove that $k \leq m_{2,3} \leq 3k - 6$. Since $m_{1,2} = k$, and the only edges incident to 2-vertices are $m_{2,2}$ and $m_{2,3}$, it follows from the structure of the tree that, regardless of the value of $m_{2,2}$, we always have

$$m_{2,3} \geq m_{1,2} = k.$$

On the other hand, from Equation (2), we have $m_{2,3} + 3m_{3,3} = 3n_3$. Given that $m_{3,3} \geq 0$ and $n_3 = k - 2$, this implies

$$m_{2,3} \leq 3k - 6.$$

Thus, the lemma is proven. ■

3 Minimal VDB topological indices of trees with given pendent vertices

In this section, we determine the minimal VDB topological indices among $\mathcal{T}_{n,k}$, and characterize those graphs that achieve the minimal values. In $\mathcal{T}_{n,k}$, have $k \geq 2$, and when $k = 2$, $\mathcal{T}_{n,2} = P_n$. Therefore, we consider trees in $\mathcal{T}_{n,k}$ such that $3 \leq k \leq \frac{n+2}{3}$, where $k \leq \frac{n+2}{3}$ follows from the expression $m_{2,2} = n - 3k + 2 \geq 0$ in Theorem 1.

Let the minimal trees of TI_f in $\mathcal{T}_{n,k}$ as follows:

$$\mathcal{T}_{n,k}^{min} = \{T \in \mathcal{T}_{n,k} : TI_f(T) \ is\ minimizing\}.$$

Recall that $g(x, y) = f(x, y) + f(3, 3) - 2f(2, 3) + 6(\frac{x+y}{xy} - 1)\big(f(3, 3) -$

$f(2,3)\big)$, and thus,

$$g(2,2) = f(2,2) + f(3,3) - 2f(2,3),$$

$$g(x,y) - g(2,2) = f(x,y) - f(2,2) + 6(\frac{x+y}{xy} - 1)\big(f(3,3) - f(2,3)\big).$$

Theorem 1. *Let* $T \in \mathcal{T}_{n,k}$ *with* $3 \le k \le \frac{n+2}{3}$*, and assume* $g(1,x) \ge g(1,2)$ *for* $x \ge 2$*.*

(i) If $g(2,2) < 0$*, and* $g(x,y) > 0$ *for any* $(x,y) \in A_2$*, then*

$$TI_f(T) \ge kf(1,2) + kf(2,3) + (k-3)f(3,3) + (n-3k+2)f(2,2),$$

the equality occurs if and only if $m_{1,2} = m_{2,3} = k$*,* $m_{3,3} = k-3$*, and* $m_{2,2} = n-3k+2$*.*

(ii) If $g(2,2) = 0$*, and* $g(x,y) > 0$ *for any* $(x,y) \in A_2$*, then*

$$\begin{aligned} TI_f(T) \ge\ & kf(1,2) + (n-4k+5+m_{3,3})f(2,2) \\ & + (3k-6-2m_{3,3})f(2,3) + m_{3,3}f(3,3), \end{aligned}$$

the equality occurs if and only if $m_{1,2} = k$*,* $m_{2,2} = n-4k+5+m_{3,3}$*,* $m_{2,3} = 3k-6-2m_{3,3}$*, and* $0 \le m_{3,3} \le k-3$*.*

(iii) If $g(2,2) > 0$*, and* $g(x,y) - g(2,2) > 0$ *for any* $(x,y) \in A_2$*, then*

$$TI_f(T) \ge kf(1,2) + (3k-6)f(2,3) + (n-4k+5)f(2,2),$$

the equality occurs if and only if $m_{1,2} = k$*,* $m_{2,3} = 3k-6$*, and* $m_{2,2} = n-4k+5$*.*

Proof. Assume $T^* \in \mathcal{T}_{n,k}^{min}$, then $\sum_x m_{1,x} = k$. From $g(1,x) \ge g(1,2)$ for $x \ge 2$ and Equation (4) of Lemma 1, to ensure the minimality of T^*, it must hold that $m_{1,2} = k$ in T^*.

(i) Let $m_{2,2} = x$. From condition (i) and Equation (4) of Lemma 1, we can derive that

$$TI_f(T) \ge (2n+4)f(2,3) - (n+5)f(3,3) + x(f(2,2) + f(3,3) - 2f(2,3))$$

$$+k(f(1,2) + f(3,3) - 2f(2,3) + 6\big(f(3,3) - f(2,3)\big)(\frac{3}{2} - 1))$$

$= kf(1,2) + (2n+4-5k-2x)f(2,3) + (x+4k-n-5)f(3,3) + xf(2,2),$

where $m_{x,y} = 0$ for all $(x,y) \in A^*\backslash\{(1,2)\}$. Now, based on the value of $x(= m_{2,2})$ in the above expression, we will determine the tree of T^*, such that $T^* \in \mathcal{T}_{n,k}^{min}$. Given that $g(2,2) = f(2,2) + f(3,3) - 2f(2,3) < 0$, the smaller $m_{2,3}$ is, the smaller the value of $TI_f(T)$ becomes. In conjunction with $m_{1,2} = k$, it follows from Lemma 2 that $m_{2,3} \geq m_{1,2} = k$. Thus, we have

$$TI_f(T) = kf(1,2)+(2n+4-5k-2x)f(2,3)+(x+4k-n-5)f(3,3)+xf(2,2)$$

$$\geq kf(1,2) + kf(2,3) + (k-3)f(3,3) + (n-3k+2)f(2,2),$$

the equality holds if and only if $m_{1,2} = m_{2,3} = k$, $m_{3,3} = k-3$, and $m_{2,2} = n-3k+2$.

(ii) Since $g(2,2) = g(2,3) = g(3,3) = 0$, to minimize the value of TI_f, we should take as many of $m_{2,2}$, $m_{2,3}$, and $m_{3,3}$ as possible in T. By condition (ii) and (4) of Lemma 1, we have

$$\begin{aligned} TI_f(T) \geq\ & (2n+4)f(2,3) - (n+5)f(3,3) \\ & + k(f(1,2) + f(3,3) - 2f(2,3) + 6\big(f(3,3) - f(2,3)\big)(\frac{3}{2} - 1)) \\ =\ & kf(1,2) + (2n+4-5k)f(2,3) + (4k-n-5)f(3,3). \end{aligned}$$

Assume $m_{3,3} = y$, we deduced by $f(2,2) + f(3,3) - 2f(2,3) = 0$ that

$$TI_f(T) \geq kf(1,2) + (3k-6-2y)f(2,3) + yf(3,3) + (n-4k+5+y)f(2,2),$$

the equality holds if and only if $m_{1,2} = k$, $m_{2,3} = 3k-6-2m_{3,3}$, and $m_{2,2} = n-4k+5+m_{3,3}$, where $0 \leq m_{3,3} \leq k-3$. Here, the upper bound $m_{3,3} \leq k-3$ is derived from $m_{2,3} = 3k-6-2m_{3,3} \geq k$ in Lemma 2.

(iii) Assume $m_{2,2} = x$. Similar to the proof of (i), we deduced by condition (iii) that

$$TI_f(T) \geq (2n+4)f(2,3) - (n+5)f(3,3) + x(f(2,2) + f(3,3) - 2f(2,3))$$

$$+k\big(f(1,2)+f(3,3)-2f(2,3)+6\big(f(3,3)-f(2,3)\big)(\frac{3}{2}-1)\big)$$

$$=kf(1,2)+(2n+4-5k-2x)f(2,3)+(x+4k-n-5)f(3,3)+xf(2,2).$$

Given the condition $g(2,2)=f(2,2)+f(3,3)-2f(2,3)>0$, it follows that the larger $m_{2,3}$ is, the smaller the value of $TI_f(T)$ becomes. Moreover, in trees containing only $m_{1,2}(=k)$, $m_{2,2}$, $m_{2,3}$, and $m_{3,3}$, Lemma 2 gives $m_{2,3}\leq 3k-6$. Therefore, when $m_{2,3}=2n+4-5k-2x=3k-6$, i.e., $x=n-4k+5$, the above expression can be transformed into

$$TI_f(T)\geq kf(1,2)+(3k-6)f(2,3)+(n-4k+5)f(2,2),$$

the equality holds if and only if $m_{1,2}=k$, $m_{2,3}=3k-6$, and $m_{2,2}=n-4k+5$. This completes the proof of the theorem. ■

Likewise, for a tree $T\in\mathcal{T}_n$ with no restriction on the number of pendent vertices, we have the following theorem.

Theorem 2. *Let $T\in\mathcal{T}_n$ with $n\geq 3$, and $g(1,x)\geq g(1,2)$ for $x\geq 2$. If one of the following conditions holds:*

(i) $g(2,2)\leq 0$, and $g(x,y)>0$ for any $(x,y)\in A_2$;

(ii) $g(2,2)>0$, and $g(x,y)-g(2,2)>0$ for any $(x,y)\in A_2$.

Then, $TI_f(T)\geq 2f(1,2)+(n-3)f(2,2)$, the equality occurs if and only if $T\cong P_n$.

Proof. For any tree T, we have $\sum_x m_{1,x}\geq 2$, the equality holds if and only if $m_{1,2}=2$ and $m_{2,2}=n-3$. Let $T^*\in\mathcal{T}_n^{min}$. From $g(1,x)\geq g(1,2)$, Equation (4) of Lemma 1, and together with the minimality of T^*, it follows that $m_{1,2}=\sum_x m_{1,x}\geq 2$ in T^*.

By the conditions of the lemma, we can easily derive that in both cases (i) and (ii), $g(2,2)<g(x,y)$ holds for all $(x,y)\in A_2$. Therefore, by combining Equation (4) of Lemma 1, we can deduce that the larger of $m_{2,2}$ is, the smaller the value of $TI_f(T)$ becomes. Thus, when $m_{2,2}=n-3$, $m_{1,2}=2$, and $m_{x,y}=0$ for all $(x,y)\in A^*\backslash\{(1,2)\}$, we obtain

$$TI_f(T)\geq(2n+4)f(2,3)-(n+5)f(3,3)+(n-3)(f(2,2)+f(3,3)$$

$$-2f(2,3))+2(f(1,2)+f(3,3)-2f(2,3)+3(f(3,3)-f(2,3)))$$

$$=2f(1,2)+(n-3)f(2,2),$$

the equality holds if and only if $m_{1,2}=2$ and $m_{2,2}=n-3$, that is $T\cong P_n$. ■

Table 1. Some VDB topological indices

No.	Indices	$f(x,y)$
1	Reciprocal sum-connectivity index	$\sqrt{x+y}$
2	Sombor index	$\sqrt{x^2+y^2}$
3	Reduced Sombor index	$\sqrt{(x-1)^2+(y-1)^2}$
4	Euler Sombor index	$\sqrt{x^2+y^2+xy}$
5	Third Sombor index	$\sqrt{2}\pi\frac{x^2+y^2}{x+y}$
6	Fourth Sombor index	$\frac{\pi}{2}(\frac{x^2+y^2}{x+y})^2$
7	First Zagreb index	$x+y$
8	Forgotten index	x^2+y^2
9	Modified first Zagreb index	$\frac{1}{x^3}+\frac{1}{y^3}$
10	Reciprocal Randič index	$\sqrt{xy}$
11	First hyper-Zagreb index	$(x+y)^2$
12	First Gourava index	$x+y+xy$
13	Product-connectivity Gourava index	$\sqrt{(x+y)xy}$
14	Exp. reciprocal sum-connectivity index	$e^{\sqrt{x+y}}$
15	Exp. inverse degree index	$e^{\frac{1}{x^2}+\frac{1}{y^2}}$

Now, we apply Theorems 1 and 2 to the VDB topological indices in Table 1. Through step-by-step calculation and verification, we can arrive at the following proposition.

Proposition 3. *(i) The VDB topological indices from No.1 to No.6 in Table 1 meet the conditions* $g(1,x)\geq g(1,2)$ *for* $x\geq 2$, $f(2,2)+f(3,3)-2f(2,3)<0$, *and* $f(x,y)+f(3,3)-2f(2,3)+6\big(f(3,3)-f(2,3)\big)(\frac{x+y}{xy}-1)>0$ *for any* $(x,y)\in A_2$*;*

(ii) The VDB topological indices from No.7 to No.10 in Table 1 meet the conditions $g(1,x)\geq g(1,2)$ *for* $x\geq 2$, $f(2,2)+f(3,3)-2f(2,3)=0$, *and* $f(x,y)+f(3,3)-2f(2,3)+6\big(f(3,3)-f(2,3)\big)(\frac{x+y}{xy}-1)>0$ *for any* $(x,y)\in A_2$*;*

(iii) The VDB topological indices from No.11 to No.16 in Table 1 meet the conditions $g(1,x) \geq g(1,2)$ *for* $x \geq 2$, $f(2,2)+f(3,3)-2f(2,3) > 0$, *and* $f(x,y)-f(2,2)+6\big(f(3,3)-f(2,3)\big)(\frac{x+y}{xy}-1) > 0$ *for any* $(x,y) \in A_2$.

Regarding the above conclusions, we only verify that the Euler Sombor index $f(x,y) = \sqrt{x^2+y^2+xy}$ in Table 1 satisfies conclusion (i). The cases involving other indices can be proven analogously and are thus omitted herein.

Proof. First, it holds that $g(2,2) = \sqrt{12}+\sqrt{27}-2\sqrt{19} \approx -0.575 < 0$.

Second, since $g(1,x) = \sqrt{x^2+x+1} + \frac{6(\sqrt{27}-\sqrt{19})}{x} + \sqrt{27}-2\sqrt{19}$, we deduce that

$$g'(1,x) = \frac{1}{\sqrt{1+\frac{\frac{3}{4}}{(x+\frac{1}{2})^2}}} - \frac{6(\sqrt{27}-\sqrt{19})}{x^2}.$$

Clearly, $g'(1,x)$ is monotonically increasing for $x \geq 3$, and thus, for $x \geq 3$, we have $g'(1,x) \geq g'(1,3) = \frac{3.5}{\sqrt{13}} - \frac{6(\sqrt{27}-\sqrt{19})}{9} \approx 0.4126 > 0$. Furthermore, given that $g(1,2) \approx 1.6358 < g(1,3) \approx 1.7584$, we can derive that $g(1,x) \geq g(1,2)$ for $x \geq 2$.

Finally, we verify that $g(x,y) > 0$ for any $(x,y) \in A_2$. Note that

$$\begin{aligned} g(x,y) &= \sqrt{x^2+y^2+xy} + \frac{x+y}{xy}(18\sqrt{3}-6\sqrt{19}) + (4\sqrt{19}-15\sqrt{3}). \\ &> \sqrt{x^2+y^2+xy} + (4\sqrt{19}-15\sqrt{3}) = h(x,y). \end{aligned}$$

For $y \geq x \geq 5$, we have $g(x,y) > h(5,5) = \sqrt{75}+4\sqrt{19}-15\sqrt{3} > 0$.

For $2 \leq x \leq 4$ and $y \geq 8$, it follows that $g(x,y) > h(2,8) > h(5,5) > 0$.

For $2 \leq x \leq 4$, $2 \leq y \leq 7$, the values of $g(x,y)$ are given in Table 2.

Thus, synthesizing the above cases, $f(x,y) = \sqrt{x^2+y^2+xy}$ satisfies conclusion (i). ■

Consequently, based on Theorems 1 and 2, we can immediately deduce the following theorems. It should further be noted that, given that all vertex degrees in the minimal tree are less than 4, these theorems apply equally to chemical trees $T \in \mathcal{CT}_{n,k}$.

Table 2. Some values of $g(x, y)$ with respect to Euler Sombor index

$g(2,4) = 2\sqrt{7} - \frac{3}{2}\sqrt{3} - \frac{1}{2}\sqrt{19} > 0$	$g(2,5) = \sqrt{39} - \frac{12}{5}\sqrt{3} - \frac{1}{5}\sqrt{19} > 0$
$g(2,6) = 2\sqrt{13} - 3\sqrt{3} > 0$	$g(2,7) = \sqrt{67} - \frac{24}{7}\sqrt{3} + \frac{1}{7}\sqrt{19} > 0$
$g(3,4) = \sqrt{37} - \frac{9}{2}\sqrt{3} + \frac{1}{2}\sqrt{19} > 0$	$g(3,5) = 7 - \frac{27}{5}\sqrt{3} + \frac{4}{5}\sqrt{19} > 0$
$g(3,6) = 3\sqrt{7} - 6\sqrt{3} + \sqrt{19} > 0$	$g(3,7) = \sqrt{79} - \frac{45}{7}\sqrt{3} + \frac{8}{7}\sqrt{19} > 0$
$g(4,4) = -2\sqrt{3} + \sqrt{19} > 0$	$g(4,5) = \sqrt{61} - \frac{69}{10}\sqrt{3} + \frac{13}{10}\sqrt{19} > 0$
$g(4,6) = -\frac{15}{2}\sqrt{3} + \frac{7}{2}\sqrt{19} > 0$	$g(4,7) = \sqrt{93} - \frac{186}{19}\sqrt{3} + \frac{43}{19}\sqrt{19} > 0$

Theorem 4. *Let $T \in \mathcal{T}_{n,k}$ (or $T \in \mathcal{CT}_{n,k}$) with $3 \le k \le \frac{n+2}{3}$.*

(i) For VDB topological indices from No.1 to No.6 in Table 1,

$$TI_f(T) \ge kf(1,2) + kf(2,3) + (k-3)f(3,3) + (n-3k+2)f(2,2),$$

the equality holds if and only if $m_{1,2} = m_{2,3} = k$, $m_{3,3} = k-3$, and $m_{2,2} = n-3k+2$.

(ii) For VDB topological indices from No.7 to No.9 in Table 1,

$$\begin{aligned} TI_f(T) \ge\ & kf(1,2) + (n-4k+5+m_{3,3})f(2,2) \\ & + (3k-6-2m_{3,3})f(2,3) + m_{3,3}f(3,3), \end{aligned}$$

the equality holds if and only if $m_{1,2} = k$, $m_{2,2} = n-4k+5+m_{3,3}$, $m_{2,3} = 3k-6-2m_{3,3}$, and $0 \le m_{3,3} \le k-3$.

(iii) For VDB topological indices from No.10 to No.15 in Table 1,

$$TI_f(T) \ge kf(1,2) + (3k-6)f(2,3) + (n-4k+5)f(2,2),$$

the equality holds if and only if $m_{1,2} = k$, $m_{2,3} = 3k-6$, and $m_{2,2} = n-4k+5$.

Theorem 5. *Let $T \in \mathcal{T}_n$ (or $T \in \mathcal{CT}_n$) with $n \ge 3$. Then, for VDB topological indices from No.1 to No.15 in Table 1,*

$$TI_f(T) \ge 2f(1,2) + (n-3)f(2,2),$$

the equality holds if and only if $T \cong P_n$.

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