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A Note on the Extremal Graphs with Respect to Vertex-Degree-Based Topological Indices for c-Cyclic Graphs

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Abstract

A general VDB topological index of G is defined as

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

where $f(x, y)$ is a real symmetric function for $x \geq 1$ and $y \geq 1$. Recently, Liu et al. (2024) presented a uniform method for solving the extremal problem with general VDB topological indices for c-cyclic graphs, which was later extended by Gao (2025) and Ali et al. (2025).

In this note, we further investigate this problem. A new mathematical formula for $\mathcal{TI}_f$ was obtained, which provided sufficient conditions for G to take its minimum value. As an application, we show that there are sixteen VDB topological indices that satisfy these conditions. In addition, we ordered six VDB topological indices for bicyclic and tricyclic graphs.

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1 Introduction

All graphs we consider are simple and connected. Let $G = (V(G), E(G))$ be a graph with vertex set $|V(G)| = n$ and edge set $|E(G)| = m$. If $m = n + c - 1$, then G is said a c-cyclic graph. In particular, if $c = 1, 2, 3$, then G is called to be a unicyclic graph, a bicyclic graph, and a tricyclic graph, respectively. If the number of maximum degree $|\Delta(G)| \leq 4$, then G is called a chemical graph. We use $\mathcal{G}_{n,c}$ ($\mathcal{CG}_{n,c}$) to denote the set of all c-cyclic graphs (chemical graphs) with order n.

Topological index is a research hotspot in the field of mathematical chemistry. Since Wiener [21] proposed the concept of the Wiener index in 1947, a large number of topological indices have been introduced, such as the ABS index [1, 2], the sum-connectivity index [8, 23], the Mostar index [3, 10], etc. Topological indices are used to indicate and predict the physicochemical properties, biological activity, and many other aspects of compounds [18,19]. Undoubtedly, the vertex-degree-based (VDB) topological indices are currently the most interesting and extensively investigated.

A general VDB topological index of G is defined as follows

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

where $f(x, y)$ is a real symmetric function for $x \geq 1$ and $y \geq 1$. For example, if $f(x) = \sqrt{x^2 + y^2 + xy}$, then

$$\mathcal{TI}_f = \sum_{uv \in E(G)} \sqrt{d(u)^2 + d(v)^2 + d(u)d(v)},$$

which is called the Euler Sombor index and was proposed independently by Gutman [12] and Tang et al. [20] in 2024. Especially, Gutman collected a few significant and well-investigated VDB topological indices in [13] .

Let $m_{i,j}$ be the number of edges in G with $(d(v_i), d(v_j)) = (i, j)$, where $v_i v_j \in E(G)$. Then

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

Due to the importance of the c-cycle graphs in chemical molecular structures, the extremum and extremal graphs of VDB topological indices over all c-cyclic graphs are one of the most investigated problems in mathematical chemistry. Deng [6] proposed a uniform method for some extremal results for Zagreb indices among unicyclic graphs and bicyclic graphs. Cruz and Rada [5] presented the minimal values of unicyclic and bicyclic graphs for the Sombor index and presented open problems for such graphs. In 2024, Das [9] completely solved these problems about unicyclic and bicyclic graphs. In 2017, Gutman [14] ordered the connected graphs with cyclomatic number $1 \leq c \leq 5$ with respect to forgotten indices. Later, Ghalavand and Ashrafi [11] ordered the connected graphs with cyclomatic number c by total irregularity. In addition, the minimal Sombor indices of chemical unicyclic graphs, chemical bicyclic graphs, and chemical tricyclic graphs are ordered by Liu et al. [16]. For more results on c-cyclic graphs, refer to references [7, 17, 22].

Recently, several scholars have attempted to use a universal method to solve the extremal problems with general VDB topological indices for c-cyclic graphs. In [17], by restricting functions $f(x, y)$ and $f(a, y) - f(b - x)$ to satisfy certain properties (such as monotonicity), sufficient conditions with the minimum VDB index for c-cyclic graphs ($c \geq 3$) are given. By transformations, Gao [15] provided a few general results for c-cyclic graphs ($c \geq 0$) having the minimum VDB index. Very recently, Ali et al. [4] have improved some restrictive conditions and provided some new sufficient conditions. Due to differences in limiting conditions, the VDB indices that satisfy the minimum value in the three papers also varies.

Inspired by these, we further investigate the extremal problems for c-circlic graphs. In Section 2, we present an important lemma that a new mathematical formula for $\mathcal{TI}_f$ are provided. From this formula, in Section 3, we obtained the minimum values of such VDB topological indices among $\mathcal{G}_{n,c}$ ($\mathcal{CG}_{n,c}$), and characterized the extremal graphs. In Section 4, as an application, we show that sixteen VDB topological indices gain the minimum values. Specifically, these results are not exactly the same as those in the previously reported. In Section 5, as another application, we ordered six VDB topological indices for bicyclic and tricyclic graphs.

2 Crucial lemma

Let $G \in \mathcal{G}_{n,c}$, and $c \in \{1, 2, \cdots, n\}$. Assume that $P = \{(x, y) \in \mathbb{N} \times \mathbb{N} : 1 \le x \le y \le n-1\} - \{(1, 1), (2, 2), (2, 3), (3, 3)\}$, $P_c = \{(x, y) \in P : x+y \le n + c\}$, and $P'_c = P_c \cup \{(2, 2), (2, 3), (3, 3)\}$. Let

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

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

Here is the important lemma that will be used in the proof of our main results.

Lemma 1. *Let $c \in \{1, 2, \cdots, n\}$, and $G \in \mathcal{G}_{n,c}$. Then*

$$TI_f(G) = \big(2f(2, 3) - f(3, 3)\big)n + \big(5f(3, 3) - 4f(2, 3)\big)(c - 1)$$
$$+g(2, 2)m_{2,2} + \sum_{(x,y)\in P_c} g(x, y)m_{x,y}, \quad (3)$$

where $g(x, y)$ is defined in (2) and $P_c = \{(x, y) \in P : x + y \le n + c\}$.

Proof. For $G \in \mathcal{G}_{n,c}$, the following relations hold

$$\sum_{(x,y)\in P'_c} \frac{x + y}{xy} m_{x,y} = n, \quad \sum_{(x,y)\in P'_c} m_{x,y} = n + c - 1.$$

They can be rewritten as

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

$$m_{2,3} + m_{3,3} = n + c - 1 - m_{2,2} - \sum_{(x,y)\in P_c} m_{x,y},$$

where $P_c = \{(x, y) \in P : x + y \le n + c\}$. The solutions of the previous equations are

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

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

Therefore, according to (1), we obtain

$$\begin{aligned}
TI_f(G) &= f(2,3)m_{2,3} + f(3,3)m_{3,3} + f(2,2)m_{2,2} + \sum_{(x,y)\in P_c} f(x,y)m_{x,y} \\
&= f(2,3)\Big(2(n-2c+2) - 2m_{2,2} + \sum_{(x,y)\in P_c} (4 - 6\frac{x+y}{xy})m_{x,y}\Big) \\
&+ f(3,3)\Big(5c - 5 - n + m_{2,2} - \sum_{(x,y)\in P_c} (5 - 6\frac{x+y}{xy})m_{x,y}\Big) \\
&+ f(2,2)m_{2,2} + \sum_{(x,y)\in P_c} g(x,y)m_{x,y} \\
&= 2f(2,3)(n-2c+2) - f(3,3)(n-5c+5) + \Big(f(2,2) + f(3,3) \\
&- 2f(2,3)\Big)m_{2,2} + \sum_{(x,y)\in P_c} \Big[f(x,y) + 6\Big(f(3,3) - f(2,3)\Big)\frac{x+y}{xy} \\
&- \Big(5f(3,3) - 4f(2,3)\Big)\Big]m_{x,y} \\
&= \Big(2f(2,3) - f(3,3)\Big)n + \Big(5f(3,3) - 4f(2,3)\Big)(c-1) \\
&+ \Big(f(2,2) + f(3,3) - 2f(2,3)\Big)m_{2,2} + \sum_{(x,y)\in P_c} \Big(f(x,y) \\
&+ 6\big(f(3,3) - f(2,3)\big)\frac{x+y}{xy} - \Big(5f(3,3) - 4f(2,3)\Big)m_{x,y} \\
&= \Big(2f(2,3) - f(3,3)\Big)n + \Big(5f(3,3) - 4f(2,3)\Big)(c-1) \\
&+ g(2,2)m_{2,2} + \sum_{(x,y)\in P_c} g(x,y)m_{x,y}.
\end{aligned}$$

This completes the proof. ■

3 Minimal VDB topological indices among $\mathcal{G}_{n,c}$ ($\mathcal{CG}_{n,c}$)

In this section, we determine the minimal VDB topological indices over $\mathcal{G}_{n,c}$ ($\mathcal{CG}_{n,c}$), and characterize those graphs that achieve the minimal values. Recall that $g(x,y) = f(x,y) + f(3,3) - 2f(2,3) + 6\big(f(3,3) - f(2,3)\big)$ $(\frac{x+y}{xy} - 1)$, and thus,

$$g(2,2) = f(2,2) + f(3,3) - 2f(2,3), \tag{4}$$

$$g(x,y) - g(2,2) = f(x,y) - f(2,2) + 6\big(f(3,3) - f(2,3)\big)(\frac{x+y}{xy} - 1). \tag{5}$$

Theorem 1. *Let $G \in \mathcal{G}_{n,1}$ with $n \geq 3$. If one of the following conditions hold:*

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

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

Then $TI_f(G) \geq nf(2,2)$, the equality occurs if and only if $G \cong C_n$.

Proof. Since $G \in \mathcal{G}_{n,1}$, $m_{2,2} \leq n$, the equality holds if and only if $G \cong C_n$. By condition (i) and (3) of Lemma 1, we deduced that

$$\begin{aligned} TI_f(G) &\geq (2f(2,3) - f(3,3))n + n(f(2,2) + f(3,3) - 2f(2,3)) \\ &= nf(2,2), \end{aligned}$$

the equality holds if and only if $G \cong C_n$.

(ii) Assume $m_{2,2} = x$. By condition (ii) and (3) of Lemma 1, we have

$$\begin{aligned} TI_f(G) &= (2f(2,3) - f(3,3))n + x(f(2,2) + f(3,3) - 2f(2,3)) \\ &= xf(2,2) + (2n - 2x)f(2,3) + (x - n)f(3,3) \\ &= x\big(f(2,2) + f(3,3) - 2f(2,3)\big) + 2nf(2,3) - nf(3,3). \end{aligned}$$

Clearly, $x - n \geq 0$ implies that $x \geq n$. This together with $g(2,2) = f(2,2) + f(3,3) - 2f(2,3) > 0$, the immediate consequence is that

$$TI_f(G) \geq nf(2,2),$$

the equality holds if and only if $x = m_{2,2} = n$, i.e., $G \cong C_n$. ■

Theorem 2. *Let $G \in \mathcal{G}_{n,2}$ (or $G \in \mathcal{CG}_{n,2}$) with $n \geq 6$.*

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

$$TI_f(G) \geq (n-4)f(2,2) + 4f(2,3) + f(3,3).$$

the equality holds if and only if $m_{2,2} = n - 4$, $m_{2,3} = 4$, *and* $m_{3,3} = 1$.

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

$$TI_f(G) \geq (n-5)f(2,2) + 6f(2,3).$$

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

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

$$TI_f(G) \geq (n-5)f(2,2) + 6f(2,3).$$

the equality holds if and only if $m_{2,2} = n - 5$, *and* $m_{2,3} = 6$.

Proof. Since $G \in \mathcal{G}_{n,2}$, $m_{2,2} \leq n-3$, the equality holds if and only if $m_{2,2} = n-3$, and $m_{2,4} = 4$.

Because of the condition (i), we have $(n-3)g(2,2) + 4g(2,4) > (n-4)g(2,2)$. Furthermore, by $m_{2,2} = n-4$ and (3) of Lemma 1, we obtain

$$\begin{aligned} TI_f(G) &\geq (2f(2,3) - f(3,3))n + (5f(3,3) - 4f(2,3)) \\ &\quad + (n-4)(f(2,2) + f(3,3) - 2f(2,3)) \\ &= (n-4)f(2,2) + 4f(2,3) + f(3,3), \end{aligned}$$

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

(ii) Similar to the proof of (i), it can be concluded by condition (ii) that if $TI_f(G)$ takes the minimal value, then $m_{2,2} \leq n-4$, and $m_{2,2} + m_{2,3} + m_{3,3} = n+1$. By (3) of Lemma 1, we deduced

$$\begin{aligned} TI_f(G) &\geq (2f(2,3) - f(3,3))n + (5f(3,3) - 4f(2,3)) \\ &= (2n-4)f(2,2) - (n-5)f(3,3), \end{aligned} \tag{6}$$

If $m_{2,2} = n-4$, by substituting $f(2,2) + f(3,3) - 2f(2,3) = 0$ into (6), we obtain

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

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

If $m_{2,2} = n-5$, we deduced by (6) that

$$TI_f(G) \geq (n-5)f(2,2) + 6f(2,3),$$

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

If $m_{2,2} \leq n-6$, by substituting $f(2,2)+f(3,3)-2f(2,3) = 0$ into (6), we deduced $m_{3,3} \leq -1$, which is a contradiction. Therefore, the conclusion (ii) of Theorem 2 holds.

(iii) Assume $m_{2,2} = x$. Since the condition $g(2,2) > 0$, and $g(x,y) > g(2,2)$ for any $(x,y) \in P_c$, it can be deduced by (3) of Lemma 1 that

$$\begin{aligned} TI_f(G) &= (2f(2,3) - f(3,3))n + 5f(3,3) - 4f(2,3) \\ &\quad + x(f(2,2) + f(3,3) - 2f(2,3)) \\ &= xf(2,2) + (2n-4-2x)f(2,3) + (5-n+x)f(3,3) \\ &= x(f(2,2) + f(3,3) - 2f(2,3)) + (2n-4)f(2,3) + (5-n)f(3,3). \end{aligned}$$

Clearly, $5-n+x \geq 0$ implies that $x \geq n-5$. This together with $g(2,2) = f(2,2) + f(3,3) - 2f(2,3) > 0$, immediately, we have

$$TI_f(G) \geq (n-5)f(2,2) + 6f(2,3),$$

the equality holds if and only if $x = m_{2,2} = n-5$, and $m_{2,3} = 6$. This completes the proof. ■

Theorem 3. *Let $G \in \mathcal{G}_{n,c}$, where $c \geq 3$, and $n \geq 5c-5$.*

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

$$TI_f(G) \geq (n-2c+1)f(2,2) + 2f(2,3) + (3c-4)f(3,3),$$

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

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

$$TI_f(G) \geq (n-5c+5+m_{3,3})f(2,2) + (6c-6-2m_{3,3})f(2,3) + m_{3,3}f(3,3),$$

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

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

$$TI_f(G) \geq (n - 5c + 5)f(2,2) + (6c - 6)f(2,3),$$

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

Proof. (i) Assume $m_{2,2} = x$. By the condition (i) and (3) of Lemma 1, we obtain

$$\begin{aligned} TI_f(G) &= (2f(2,3) - f(3,3))n + (5f(3,3) - 4f(2,3))(c-1) \\ &\quad + x(f(2,2) + f(3,3) - 2f(2,3)) \\ &= x(f(2,2) + f(3,3) - 2f(2,3)) + (2n - 4c + 4)f(2,3) \\ &\quad + (5c - 5 - n)f(3,3). \end{aligned}$$

Clearly, $m_{2,3} = 2n - 4c + 4 - 2x \geq 2$ implies that $x \geq n - 2c + 1$. As $f(2,2) + f(3,3) - 2f(2,3) < 0$, then we have

$$TI_f(G) \geq (n - 2c + 1)f(2,2) + 2f(2,3) + (3c - 4)f(3,3),$$

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

(ii) By the condition (ii) and (3) of Lemma 1, we have

$$\begin{aligned} TI_f(G) &= (2f(2,3) - f(3,3))n + (5f(3,3) - 4f(2,3))(c-1) + 0 \\ &= (2n - 4c + 4)f(2,3) + (5c - 5 - n)f(3,3). \end{aligned}$$

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

$$\begin{aligned} TI_f(G) &\geq ((2n - 4c + 4) + 2(5c - 5 - n - y))f(2,3) \\ &\quad + yf(3,3) - (5c - 5 - n - y)f(2,2) \\ &= (n - 5c + 5 + y)f(2,2) + (6c - 6 - 2y)f(2,3) + yf(3,3). \end{aligned}$$

The fact $m_{2,3} = 6c - 6 - 2y \geq 2$ implies that $y \leq 3c - 4$. Therefore, the equality holds if and only if $m_{2,2} = n - 5c + 5 + m_{3,3}$, $m_{2,3} = 6c - 6 - 2m_{3,3}$, and $0 \leq m_{3,3} \leq 3c - 4$.

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

$$\begin{aligned} TI_f(G) &= (2f(2,3) - f(3,3))n + (5f(3,3) - 4f(2,3))(c-1) \\ &\quad + x(f(2,2) + f(3,3) - 2f(2,3)) \\ &= x(f(2,2) + f(3,3) - 2f(2,3)) + (2n - 4c + 4)f(2,3) \\ &\quad + (5c - 5 - n)f(3,3). \end{aligned}$$

Clearly, $(5c - 5 - n + x) \geq 0$ implies that $x \geq n - 5c + 5$. Consequently, we have

$$TI_f(G) \geq (n - 5c + 5)f(2,2) + (6c - 6)f(2,3),$$

the equality holds if and only if $x = m_{2,2} = n - 5c + 5$, $m_{2,3} = 6c - 6$. ■

4 Applications in minimal c-cyclic graphs ($\mathcal{CG}_{n,c}$)

In this section, we consider the VDB topological indices in Table 1. It is not difficult to verify the following conclusions.

(i) The VDB topological indices from No.1 to No.6 in Table 1 satisfy the condition $f(2,2) + f(3,3) - 2f(2,3) < 0$, 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 $(x,y) \in P_c$;

(ii) The VDB topological indices from No.7 to No.10 in Table 1 satisfy the condition $f(2,2)+f(3,3)-2f(2,3) = 0$, 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 $(x,y) \in P_c$;

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

Consequently, by Theorems 1, 2, and 3, we deduce the following theorems immediately.

Theorem 4. *Let $G \in \mathcal{G}_{n,1}$ (or $G \in \mathcal{CG}_{n,1}$) with $n \geq 3$. For all VDB topological indices in Table 1,*

$$TI_f(G) \geq nf(2,2),$$

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	Inverse degree index	$\frac{1}{x^2}+\frac{1}{y^2}$
10	Modified first Zagreb index	$\frac{1}{x^3}+\frac{1}{y^3}$
11	Reciprocal Randič index	$\sqrt{xy}$
12	First hyper-Zagreb index	$(x+y)^2$
13	First Gourava index	$x+y+xy$
14	Product-connectivity Gourava index	$\sqrt{(x+y)xy}$
15	Exp. reciprocal sum-connectivity index	$e^{\sqrt{x+y}}$
16	Exp. inverse degree index	$e^{\frac{1}{x^2}+\frac{1}{y^2}}$

the equality occurs if and only if $G \cong C_n$.

Theorem 5. *Let* $G \in \mathcal{G}_{n,2}$ *(or* $G \in \mathcal{CG}_{n,2}$*) with* $n \geq 6$.

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

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

the equality holds if and only if $m_{2,2} = n-4$, $m_{2,3} = 4$, *and* $m_{3,3} = 1$.

(ii) For VDB topological indices from No.1 to No.7 in Table 10,

$$TI_f(G) \geq (n-5)f(2,2) + 6f(2,3),$$

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

(iii) For VDB topological indices from No.11 to No.16 in Table 1,

$$TI_f(G) \geq (n-5)f(2,2) + 6f(2,3).$$

the equality holds if and only if $m_{2,2} = n - 5$*, and* $m_{2,3} = 6$*.*

Theorem 6. *Let* $G \in \mathcal{G}_{n,c}$ *(or* $G \in \mathcal{CG}_{n,c}$*) with* $c \geq 3$ *and* $n \geq 5c - 5$*.*

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

$$TI_f(G) \geq (n - 2c + 1)f(2,2) + 2f(2,3) + (3c - 4)f(3,3),$$

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

(ii) For VDB topological indices from No.1 to No.7 in Table 10,

$$TI_f(G) \geq (n - 5c + 5 + m_{3,3})f(2,2) + (6c - 6 - 2m_{3,3})f(2,3) + m_{3,3}f(3,3),$$

the equality holds if and only if $m_{2,2} = n - 5c + 5 + m_{3,3}$*,* $m_{2,3} = 6c - 6 - 2m_{3,3}$*, and* $0 \leq m_{3,3} \leq 3c - 4$*.*

(iii) For VDB topological indices from No.11 to No.16 in Table 1,

$$TI_f(G) \geq (n - 5c + 5)f(2,2) + (6c - 6)f(2,3),$$

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

5 Applications in ordering bicyclic and tricyclic graphs (chemical graphs)

In this section, as another application of Lemma 1, we determine more extremal bicyclic and tricyclic graphs (chemical graphs) for VDB topological indices from No.1 to No.6 in Table 1.

Theorem 7. *Let* $G, G_1, G_2 \in \mathcal{G}_{n,2}$ *(or* $\mathcal{CG}_{n,2}$*) with* $n \geq 6$*. If* $G_1 \in \alpha_1$*,* $G_2 \in \alpha_2$ *in Table 2, and* $\Gamma \in \mathcal{G}_{n,2} \backslash \{G_1, G_2\}$*. Then, for VDB topological indices from No.1 to No.6 in Table 1,*

$$TI_f(G_1) < TI_f(G_2) < TI_f(\Gamma).$$

Proof. By Section 4, we verified that $g(2,2) < 0$, and $g(x,y) > 0$ for any $(x,y) \in P_c$ for VDB topological indices from No.1 to No.6 in Table 1. Since

Table 2. Bicyclic graphs α_i and tricyclic graphs β_j

Graphs	$m_{2,2}$	$m_{2,3}$	$m_{3,3}$
α_1	$n-4$	4	1
α_2	$n-5$	6	0
β_1	$n-5$	5	2
β_2	$n-6$	4	4
β_3	$n-7$	6	3
β_4	$n-8$	8	2
β_5	$n-9$	10	1
β_6	$n-10$	12	0

$G \in \mathcal{G}_{n,2}$, $m_{2,3} \leq n-3$, the equality holds if and only if $m_{2,3} = n-3$, and $m_{2,4} = 4$.

By Theorem 5, $TI_f(G_1) \leq TI_f(G)$, the equality holds if and only if $m_{2,2} = n-4$, $m_{2,3} = 4$, and $m_{3,3} = 1$. Let $m_{2,2} = x$, where $x \leq n-5$. Using (3) of Lemma 1, we obtain

$$\begin{aligned} TI_f(G) &= (2f(2,3) - f(3,3))n + \Big(5f(3,3) - 4f(2,3)\Big) \\ &\quad + x(f(2,2) + f(3,3) - 2f(2,3)) \\ &= xf(2,2) + (2n-2x-4)f(2,3) + (x-n+5)f(3,3), \end{aligned}$$

If $m_{2,2} = n-5$, then $TI_f(G) = (n-5)f(2,2) + 6f(2,3) = TI_f(G_2)$.

If $m_{2,2} \leq n-6$, then $m_{3,3} \leq -1$, a contradiction.

On the other hand, as $(n-3)g(2,2) + 4g(2,4) > (n-5)g(2,2) > (n-4)g(2,2)$, then

$$TI_f(G_1) < TI_f(G_2) < TI_f(\Gamma).$$

This completes the proof. ■

Theorem 8. *Let $G, G_1, G_2, \cdots, G_6 \in \mathcal{G}_{n,3}$ (or $\mathcal{CG}_{n,3}$) with $n \geq 6$. If $G_j \in \beta_j$ for $1 \leq j \leq 6$ in Table 2, and $\Gamma \in \mathcal{G}_{n,3} \backslash \{G_1, G_2, \cdots, G_6\}$. Then, for VDB topological indices from No.1 to No.6 in Table 1,*

$$TI_f(G_1) < TI_f(G_2) < TI_f(G_3) < TI_f(G_4) < TI_f(G_5) < TI_f(G_6) < TI_f(\Gamma).$$

Proof. By Section 4, we verified that $g(2,2) < 0$, and $g(x,y) > 0$ for any $(x,y) \in P_c$ for VDB topological indices from No.1 to No.6 in Table 1. Since $G \in \mathcal{G}_{n,3}$, $m_{2,3} \leq n-4$, the equality holds if and only if $m_{2,3} = n-4$, and $m_{2,6} = 6$.

By Theorem 6, $TI_f(G_1) \leq TI_f(G)$, the equality holds if and only if $m_{2,2} = n-5$, $m_{2,3} = 2$, and $m_{3,3} = 5$. Let $m_{2,2} = x$, where $x \leq n-6$. Using (3) of Lemma 1, we obtain

$$\begin{aligned} TI_f(G) &= (2f(2,3) - f(3,3))n + 2\Big(5f(3,3) - 4f(2,3)\Big) \\ &\quad + x(f(2,2) + f(3,3) - 2f(2,3)) \\ &= xf(2,2) + (2n-2x-8)f(2,3) + (x-n+10)f(3,3), \end{aligned}$$

If $m_{2,2} = n-6$, then $TI_f(G) = (n-6)f(2,2) + 4f(2,3) + 4f(2,3) = TI_f(G_2)$.

If $m_{2,2} = n-7$, then $TI_f(G) = (n-7)f(2,2) + 6f(2,3) + 3f(2,3) = TI_f(G_3)$.

If $m_{2,2} = n-8$, then $TI_f(G) = (n-8)f(2,2) + 8f(2,3) + 2f(2,3) = TI_f(G_4)$.

If $m_{2,2} = n-9$, then $TI_f(G) = (n-9)f(2,2) + 10f(2,3) + f(2,3) = TI_f(G_5)$.

If $m_{2,2} = n-10$, then $TI_f(G) = (n-10)f(2,2) + 12f(2,3) = TI_f(G_6)$.

If $m_{2,2} \leq n-11$, then $m_{3,3} \leq -1$, a contradiction.

On the other hand, as $g(2,2) < 0$ and $g(2,4) > 0$, thus

$$(n-4)g(2,2) + 6g(2,4) > (n-10)g(2,2) > (n-9)g(2,2)$$

$$> (n-8)g(2,2) > (n-7)g(2,2) > (n-6)g(2,2) > (n-5)g(2,2).$$

Consequently,

$$TI_f(G_1) < TI_f(G_2) < TI_f(G_3) < TI_f(G_4) < TI_f(G_5) < TI_f(G_6) < TI_f(\Gamma).$$

This completes the proof. ■

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References

[1] A. Ali, B. Furtula, I. Redžepović, I. Gutman, Atom-bond sum-connectivity index, *J. Math. Chem.* **60** (2022) 2081–2093.

[2] A. Ali, I. Gutman, B. Furtula, I. Redžepović, T. Došlić, Z. Razae, Extremal results and bounds for atom-bond sum-connectivity index, *MATCH Commun. Math. Comput. Chem.* **92** (2024) 271–314.

[3] A. Ali, T. Došlić, Mostar index: Results and perspectives, *Appl. Math. Comput.* **404** (2021) #126245.

[4] A. Ali, D. Dimitrov, T. Reti, A. M. Alotaibi, A. M. Alanazi, T. S. Hassan, Degree-based graphical indices of k-cyclic graphs, *AIMS Math.* **10** (2025) 13540–13554.

[5] R. Cruz, J. Rada, Extremal values of the Sombor index in unicyclic and bicyclic graphs, *J. Math. Chem.* **59** (2021) 1098–1116.

[6] H. Deng, A unified approach to the extremal Zagreb indices for trees, unicyclic graphs and bicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 597–616.

[7] H. Deng, S. Elumalai, S. Balachandran, Maximum and second maximum of geometric-arithmetic index of tricyclic graphs, *MATCH Commun. Math. Comput. Chem.* **79** (2018) 467–475.

[8] K. C. Das, S. Das, B. Zhou, Sum-connectivity index of a graph, *Front. Math. China.* **11** (2016) 47–54.

[9] K. C. Das, Open problems on Sombor index of unicyclic and bicyclic graphs, *Appl. Math. Comput.* **473** (2024) #128647.

[10] T. Došlić, I. Martinjak, R. Škrekovski, S. Tipurić Spužević, I. Zubac, Mostar index, *J. Math. Chem.* **56** (2018) 2995–3013.

[11] A. Ghalavand, A. R. Ashrafi, Ordering of c-cyclic graphs with respect to total irregularity, *J. Appl. Math. Comput.* **63** (2020) 707–715.

[12] I. Gutman, Relating Sombor and Euler indices, *Vojnoteh. Glas.* **72** (2024) 1–12.

[13] I. Gutman, Geometric approach to vertex-degree-based topological indices: Sombor indices, *MATCH Commun. Math. Comput. Chem.* **86** (2021) 11–16.

[14] I. Gutman, A. Ghalavand, T. Dehghan-Zadeh, A. R. Ashrafi, Graphs with smallest forgotten index, *Iran. J. Math. Chem.* **8** (2017) 259–273.

[15] W. Gao, Extremal graphs with respect to vertex-degree-based topological indices for c-cyclic graphs, *MATCH Commun. Math. Comput. Chem.* **93** (2025) 549–566.

[16] H. Liu, L. You, Y. Huang, Ordering chemical graphs by Sombor indices and its applications, *MATCH Commun. Math. Comput. Chem.* **87** (2022) 5–22.

[17] H. Liu, Z. Du, Y. Huang, H. Chen, S. Elumalai, Note on the minimum bond incident degree indices of k-cyclic graphs, *MATCH Commun. Math. Comput. Chem.* **91** (2024) 255–266.

[18] I. Redžepović, Chemical applicability of Sombor indices, *J. Serb. Chem. Soc.* **86** (2021) 445–457.

[19] R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Wiley-VCH, Weinheim, 2000.

[20] Z. Tang, Y. Li, H. Deng, The Euler Sombor index of a graph, *Int. J. Quantum Chem.* **124** (2024) #e27387.

[21] H. Wiener, Structural determination of paraffin boiling points, *J. Amer. Chem. Soc.* **69** (1947) 17–20.

[22] Y. Yao, M. Liu, K. C. Das, Y. Ye, Some extremal results for vertex-degree-based invariants, *MATCH Commun. Math. Comput. Chem.* **81** (2019) 325–344.

[23] B. Zhou, N. Trinajstić, On a novel connectivity index, *J. Math. Chem.* **46** (2009) 1252–1270.