ON THE GENERAL VERTEX-DEGREE-BASED INDEX OF CHEMICAL TREES WITH GIVEN BRANCHING VERTICES

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The general sum-connectivity index and the general Sombor index have gained significant attention in recent years. In this study, we consider a more generalized form of these indices, denoted by $\mathcal{KD}_{\alpha,\beta}$. For a graph G, this index is defined as

$$\mathcal{KD}_{\alpha,\beta}(G) = \sum_{xy\in E(G)} \left(d_G(x)^{\beta} + d_G(y)^{\beta}\right)^{\alpha},$$

where α and β are nonzero real numbers. This paper establishes an upper bound on $\mathcal{KD}_{\alpha,\beta}$ for chemical trees with given order n and branching vertices $b \geq 1$, where $\alpha \in (0, 1]$ and $\beta > 0$. We also characterize the maximal chemical trees. Since the general sum-connectivity index is a special case of $\mathcal{KD}_{\alpha,\beta}$ with $\beta = 1$, our results generalize the findings of the first Zagreb index in S. Noureen et al. [MATCH Commun. Math. Comput. Chem. 84 (2020), 513–534]. Similarly, since the general Sombor index corresponds to $\beta = 2$, our results extend the findings for the Sombor index in A. Ali et al. [AIMS Math. 8 (2023), 5369–5390].

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1. INTRODUCTION

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. The degree of a vertex $x \in V(G)$ in G is denoted by $d_G(x)$ and the set of vertices adjacent to x is denoted by $N_G(x)$. A vertex in graph G with degree at least three is called a branching vertex. A degree sequence is a sequence that lists the degrees of the vertices in a graph G in non-increasing order, denoted by $D(G) = \pi(G) = (d_1, d_2, \ldots, d_n)$.

The graph $G - xy$ is obtained from G by removing an edge $xy \in E(G)$, while $G + xy$ is obtained from G by adding an edge $xy \notin E(G)$. An n-vertex tree with $n-1$ pendent vertices is called a star, denoted by S_n. The double star graph $DS_{p,q}$ is a tree with exactly two non-pendant vertices that are adjacent

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by an edge, one with degree p and the other with degree q. A tree in which the degree of each vertex is at most 4 is called a chemical tree. The total number of vertices with degree i in a tree T is denoted by $n_i(T)$ (or n_i), and the number of edges between vertices of degree i and j is denoted by $m_{ij}(T)$ (or simply m_{ij}).

In chemical graph theory, a topological index is a mathematical measure that describes the topological properties of a molecule. Numerous vertex-degree-based (VDB) graph indices have been put forward and thoroughly examined in the literature on mathematical chemistry.

Among the several hundred presently existing graph-based molecular structure descriptors, the variants of the Randić index [29] are certainly the most widely applied in chemistry and pharmacology. One is the general sum-connectivity index [37], which generalizes the sum-connectivity index [36] and the first Zagreb index [19]. Motivated by the generalization of Randić and sum-connectivity indices, as well as extensive studies on the Sombor index, the general Sombor index was recently introduced in [21]. The geometric interpretation of the Sombor index has garnered significant attention in a short time, leading to a notable volume of research [5–11, 13, 15, 26, 30] and several generalized versions appearing in the literature [20, 21, 31].

In this study, we consider a more generalized form of these indices, denoted by $\mathcal{KD}_{\alpha,\beta}$. For a graph G, this index is defined as in [20]

$$\mathcal{KD}_{\alpha,\beta}(G) = \sum_{xy \in E(G)} \left(d_G(x)^\beta + d_G(y)^\beta\right)^\alpha,$$

where α and β are nonzero real numbers. In this paper, we study a class of topological indices derived from the $\mathcal{KD}_{\alpha,\beta}$ index by introducing parameters α and β. Such generalizations are important in chemical graph theory because they extend the applicability of a topological index while preserving its fundamental characteristics. The following table presents various topological indices derived from the $\mathcal{KD}_{\alpha,\beta}$ index for different values of α and β.

For recent research on various generalizations of the Sombor index, see [2, 12, 20, 27, 31, 32, 34, 35], and for the chemical applications of the general Sombor index, refer to [1]. In the literature, various topological indices have been discussed, as highlighted in [4, 14, 33].

In this paper, we focus on finding the upper bound for chemical trees of order n with $b \geq 1$ branching vertices with respect to $\mathcal{KD}_{\alpha,\beta}$ index when $\alpha \in (0, 1]$ and $\beta > 0$. Within these intervals of α and β, many well-known indices emerge, and thus our results also hold for these indices. Our focus in this paper is on chemical trees; therefore, for a chemical tree T, the following

α, β	$\mathcal{KD}_{\alpha,\beta}$	name
$\alpha \neq 0,\ \beta = 1$	$\mathcal{KD}_{\alpha,1} = \mathcal{X}_\alpha$ [37]	general sum-connectivity
$\alpha = -1,\ \beta = 1$	$2\,\mathcal{KD}_{-1,1} = \mathcal{H}$ [16]	harmonic index
$\alpha = -\frac{1}{2},\ \beta = 1$	$\mathcal{KD}_{-\frac{1}{2},1} = \mathcal{X}$ [36]	sum-connectivity index
$\alpha = 1,\ \beta = 1$	$\mathcal{KD}_{1,1} = \mathcal{M}_1$ [19]	first Zagreb index
$\alpha \neq 0,\ \beta = 2$	$\mathcal{KD}_{\alpha,2} = \mathcal{SO}_\alpha$ [21]	general Sombor index
$\alpha = \frac{1}{2},\ \beta = 2$	$\mathcal{KD}_{\frac{1}{2},2} = \mathcal{SO}$ [18]	Sombor index
$\alpha = 1,\ \beta = 2$	$\mathcal{KD}_{1,2} = \mathcal{F}$ [17]	forgotten index
$\alpha = \frac{1}{2},\ \beta = 1$	$\mathcal{KD}_{\frac{1}{2},1} = \mathcal{N}$ [22]	Nirmala index
$\alpha = -\frac{1}{2},\ \beta = 2$	$\mathcal{KD}_{-\frac{1}{2},2} = \mathcal{SO}^m$ [24]	modified Sombor index
$\alpha = -2,\ \beta = \frac{1}{2}$	$\mathcal{KD}_{-2,\frac{1}{2}} = \mathcal{BSO}$ [23]	Banhatti–Sombor index

Table 1 – Degree-based indices derived from specific values of α and β in $\mathcal{KD}_{\alpha,\beta}$, showcasing its versatility.

results are well known:

$$n = \sum_{i=1}^{4} n_i(T), \tag{1}$$

$$2(n-1) = \sum_{i=1}^{4} i n_i(T), \text{ and} \tag{2}$$

$$i n_i(T) = 2m_{ii}(T) + \sum_{\substack{j=1 \\ j\neq i}}^{4} m_{ij}(T), \quad 1 \leq i \leq 4. \tag{3}$$

Assume $\mathcal{CT}_{n,b}$ is the class of chemical tress of given order $n \geq 2b+2$ with $b \geq 1$ branching vertices. For $n < 2b+2$, there are no graphs in $\mathcal{CT}_{n,b}$ for $b \geq 1$. For $n = 4$ and $b = 1$, we have $\mathcal{CT}_{4,1} = \{S_4\}$, while for $n = 5$ and $b = 1$, $\mathcal{CT}_{4,1} = \{S_5, DS_{4,2}\}$. For $n \geq 6$ and $b \geq 1$, we partition $\mathcal{CT}_{n,b}$ into two subclasses, namely $\mathcal{CT}'_{n,b}$ and $\mathcal{CT}''_{n,b}$, defined as

$$\mathcal{CT}'_{n,b} = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3 \cup \Gamma_4 \text{ and } \mathcal{CT}''_{n,b} = \Gamma_5 \cup \Gamma_6 \cup \Gamma_7,$$

where

$$\Gamma_1 = \left\{T \in \mathcal{CT}_{n,b} \mid n = 13 \text{ and } b = 4\right\},$$

$$\Gamma_2 = \left\{ T \in \mathcal{CT}_{n,b} \mid 2b+2 \le n \le \left\lfloor \frac{5b+5}{2} \right\rfloor \text{ and } b \ge 2 \right\},$$
$$\Gamma_3 = \left\{ T \in \mathcal{CT}_{n,b} \mid \left\lceil \frac{5b+6}{2} \right\rceil \le n \le \left\lfloor \frac{8b+7}{3} \right\rfloor \text{ and } b \ge 6 \right\},$$
$$\Gamma_4 = \left\{ T \in \mathcal{CT}_{n,b} \mid \left\lceil \frac{8b+8}{3} \right\rceil \le n \le 3b+2 \text{ and } b \ge 2 \right\},$$
$$\Gamma_5 = \left\{ T \in \mathcal{CT}_{n,b} \mid n \ge 3b+3 \text{ and } b = 1 \right\},$$
$$\Gamma_6 = \left\{ T \in \mathcal{CT}_{n,b} \mid 3b+3 \le n \le 4b+1 \text{ and } b \ge 2 \right\},$$
$$\Gamma_7 = \left\{ T \in \mathcal{CT}_{n,b} \mid n \ge 4b+2 \text{ and } b \ge 2 \right\}.$$

For example, see T_1, T_2, $T_3 \in \Gamma_1$, T_4, T_5, $T_6 \in \Gamma_2$, T_7, T_8, $T_9 \in \Gamma_3$, T_{10}, T_{11}, $T_{12} \in \Gamma_4$, T_{13}, T_{14}, $T_{15} \in \Gamma_5$, T_{16}, T_{17}, $T_{18} \in \Gamma_6$ and T_{19}, T_{20}, $T_{21} \in \Gamma_7$ in Figure 1.

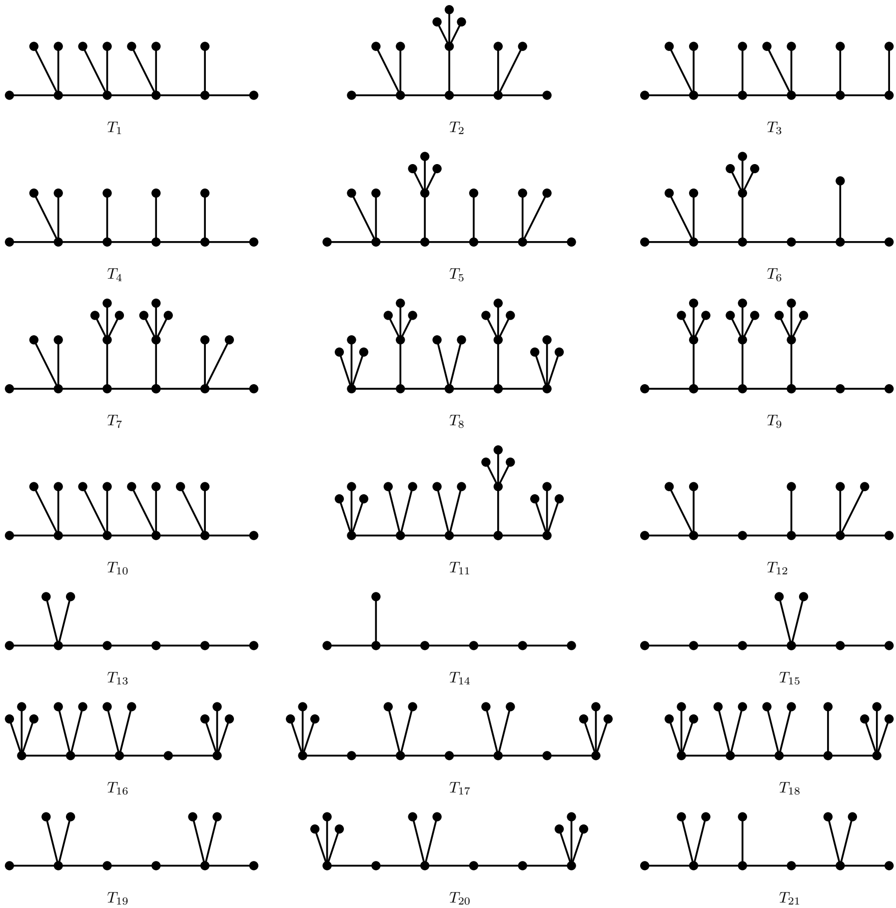


Figure 1 – Twenty-one trees $T_1, T_2, T_3, \ldots, T_{21}$.

When $b \geq 2$, the interval $2b+2 \leq n \leq 3b+2$ is further segmented into three sub-intervals, ensuring no overlap. The sub-intervals $2b+2 \leq n \leq \lfloor \frac{5b+5}{2} \rfloor$ and $\lceil \frac{8b+8}{3} \rceil \leq n \leq 3b+2$, cover most cases where $b \geq 2$. On the other hand, commencing the sub-interval $\lceil \frac{5b+6}{2} \rceil \leq n \leq \lfloor \frac{8b+7}{3} \rfloor$ from $b \geq 6$ ensures thorough coverage, excluding the cases where $b < 6$ because the domain for $b < 6$ is covered in $\lceil \frac{8b+8}{3} \rceil \leq n \leq 3b+2$. Notably, a chemical tree in $\mathcal{CT}'_{n,b}$ with $n = 13$ and $b = 4$ does not align with any of this classification. Therefore, we discuss this case separately in Lemma 2.4.

In the following section, we derive the upper bounds for chemical trees in $\mathcal{CT}_{n,b}$ with respect to the $\mathcal{KD}_{\alpha,\beta}$ index when $\alpha \in (0,1]$ and $\beta > 0$, and also construct the chemical trees that achieve these upper bounds.

2. BEST POSSIBLE UPPER BOUNDS FOR CHEMICAL TREES IN $\mathcal{CT}_{n,b}$ WITH RESPECT TO THE $\mathcal{KD}_{\alpha,\beta}$ INDEX

This section aims to find the extremal chemical trees in $\mathcal{CT}_{n,b}$ with the highest value of the $\mathcal{KD}_{\alpha,\beta}$ index when $\alpha \in (0,1]$ and $\beta > 0$. To prove the results, we first need the following lemmas. Lemma 2.1 plays a crucial role in establishing the subsequent results.

LEMMA 2.1. *Let z, c, d, α and β be real numbers, where $c,\ d > 0$, $z > 0$, $\alpha \in (0,1]$ and $\beta > 0$. Consider a function*

$$f_{c,\,d}(z) = (z^{\beta} + c^{\beta})^{\alpha} - (z^{\beta} + d^{\beta})^{\alpha}.$$

(i) *If $c > d$ and $\alpha \in (0,1]$, then $f_{c,d}(z)$ is a decreasing function. Moreover, if $c > d$ and $\alpha \in (0,1)$, then $f_{c,d}(z)$ is a strictly decreasing function.*

(ii) *If $c < d$ and $\alpha \in (0,1]$, then $f_{c,d}(z)$ is strictly increasing. Moreover, if $c < d$ and $\alpha \in (0,1)$, then $f_{c,d}(z)$ is a strictly increasing function.*

Proof. We obtain

$$f'_{c,d}(z) = \alpha\beta\, z^{\beta-1}\big[(z^{\beta} + c^{\beta})^{\alpha-1} - (z^{\beta} + d^{\beta})^{\alpha-1}\big].$$

(i) Since $c > d$, $\alpha \in (0,1]$ and $\beta > 0$, it follows that

$$(z^{\beta} + c^{\beta})^{\alpha-1} \leq (z^{\beta} + d^{\beta})^{\alpha-1}.$$

This means $f'_{c,\,d}(z) \leq 0$. Thus $f_{c,\,d}(z)$ is a decreasing function on $c > d$, $\alpha \in (0,1]$ and $\beta > 0$. Similarly, for $c > d$ and $\alpha \in (0,1)$, one can easily see that $f_{c,\,d}(z)$ is a strictly decreasing function.

(ii) By reversing the function, the proof is similar to the proof of (i). □

We define the degree sequence $\pi_1(T)$ as follows:

$$\pi_1(T) = (\underbrace{4, \ldots, 4}_{n-2(b+1)}, \underbrace{3, \ldots, 3}_{3b-n+2}, \underbrace{1, \ldots, 1}_{n-b}). \tag{4}$$

Now, we prove the following lemmas to establish the main theorem.

Lemma 2.2. *Let $T \in \mathcal{CT}'_{n,b}$ $(n \geq 6)$ be a chemical tree that maximizes the $\mathcal{KD}_{\alpha,\beta}$ index for $\alpha \in (0,1]$ and $\beta > 0$. Then T has the degree sequence $\pi_1(T)$ defined in (4).*

Proof. On the contrary, assume that $n_2 \geq 1$. Then T contains a vertex $w \in V(T)$ such that $d_T(w) = 2$. Let $N_T(w) = \{w_1, w_2\}$. If $n_3 = 0$, then from (1) and (2), we obtain $n_1 = 2 + 2n_4$. Using this, (1) gives $n \geq 3b+3$, a contradiction as $T \in \mathcal{CT}'_{n,b}$. Otherwise, $n_3 \geq 1$. Thus there exists a vertex $x \in V(T)$ such that $d_T(x) = 3$. Let $N_T(x) = \{x_1, x_2, x_3\}$. Without loss of generality, assume that points x_1 and w_1 lie on the $x - w$ path in T (w_1 and x_1 may coincide). This gives $2 \leq d_T(x_1)$, $d_T(w_1) \leq 4$ and $1 \leq d_T(x_2)$, $d_T(x_3), d_T(w_2) \leq 4$. Now we construct a tree T' from T as follows:

$$T' = T - ww_2 + xw_2.$$

Then we see that $d_{T'}(x) = d_T(x) + 1 = 4$, $d_{T'}(w) = d_T(w) - 1 = 1$ and $d_{T'}(t) = d_T(t)$ for all $t \in V(T) \setminus \{x, w\}$. Now we discuss two possibilities.

Case 1. w and x are not adjacent (w_1 and x_1 may coincide). Then

$$\begin{aligned}
&\mathcal{KD}_{\alpha,\beta}(T') - \mathcal{KD}_{\alpha,\beta}(T)\\
&\quad= \sum_{i=2}^{3}\left((4^\beta + d_T(x_i)^\beta)^\alpha - (3^\beta + d_T(x_i)^\beta)^\alpha\right) + \left(4^\beta + d_T(x_1)^\beta\right)^\alpha\\
&\qquad - \left(3^\beta + d_T(x_1)^\beta\right)^\alpha + \left(4^\beta + d_T(w_2)^\beta\right)^\alpha - \left(2^\beta + d_T(w_2)^\beta\right)^\alpha\\
&\qquad + \left(1^\beta + d_T(w_1)^\beta\right)^\alpha - \left(2^\beta + d_T(w_1)^\beta\right)^\alpha\\
&\quad> \left(4^\beta + d_T(w_2)^\beta\right)^\alpha - \left(2^\beta + d_T(w_2)^\beta\right)^\alpha + \left(1^\beta + d_T(w_1)^\beta\right)^\alpha\\
&\qquad - \left(2^\beta + d_T(w_1)^\beta\right)^\alpha.
\end{aligned}$$

By using Lemma 2.1 (i) and (ii), we obtain

$$\begin{aligned}
\mathcal{KD}_{\alpha,\beta}(T') - \mathcal{KD}_{\alpha,\beta}(T) &> (2\cdot 4^\beta)^\alpha - (2^\beta + 4^\beta)^\alpha + (1 + 2^\beta)^\alpha - (2\cdot 2^\beta)^\alpha\\
&= (2^{\alpha\beta} - 1)\left[(2\cdot 2^\beta)^\alpha - (1 + 2^\beta)^\alpha\right] > 0,
\end{aligned}$$

since $2^{\alpha\beta} > 1$ for $\alpha, \beta > 0$, it follows that $2^{\alpha\beta} - 1 > 0$ and

$$(2\cdot 2^\beta)^\alpha = 2^{(\beta+1)\,\alpha} > (1 + 2^\beta)^\alpha.$$

So $\mathcal{KD}_{\alpha,\beta}(T') > \mathcal{KD}_{\alpha,\beta}(T)$, leads to a contradiction.

Case 2. w and x are adjacent. Then

$$\begin{aligned}\mathcal{KD}_{\alpha,\beta}(T') - \mathcal{KD}_{\alpha,\beta}(T) &= \sum_{i=2}^{3}\big((4^\beta + d_T(x_i)^\beta)^\alpha - (3^\beta + d_T(x_i)^\beta)^\alpha\big) \\ &\quad + \big(4^\beta + d_T(w_2)^\beta\big)^\alpha - \big(2^\beta + d_T(w_2)^\beta\big)^\alpha \\ &> 0.\end{aligned}$$

Thus, a contradiction arises from each case. Consequently, $n_2(T) = 0$.

Now by using $n_2 = 0$ in (1) and (2), and solving them simultaneously, we obtain the degree sequence

$$\pi_1(T) = (\underbrace{4, \ldots, 4}_{n-2b-2}, \underbrace{3, \ldots, 3}_{3b+2-n}, \underbrace{1, \ldots, 1}_{n-b}).$$

This completes the proof. □

The following corollary is a direct consequence of Lemma 2.2.

COROLLARY 2.3. *Let $T \in \mathcal{CT}'_{n,b}$ ($n \geq 6$) be a chemical tree that maximizes the $\mathcal{KD}_{\alpha,\beta}$ index for $\alpha \in (0,1]$ and $\beta > 0$. Then $n_2 = 0$, that is, $m_{12} = m_{22} = m_{23} = m_{24} = 0$.*

LEMMA 2.4. *Let $T \in \Gamma_1$ be a chemical tree that maximizes the $\mathcal{KD}_{\alpha,\beta}$ index for $\alpha \in (0,1)$ and $\beta > 0$. Then* (i) *$n_1 = 9$, $n_2 = 0$, $n_3 = 1$, $n_4 = 3$,* (ii) *$m_{33} = 0$,* (iii) *$m_{44} = 0$,* (iv) *$m_{13} = 0$, $m_{14} = 9$ and $m_{34} = 3$.*

Proof. Since $T \in \Gamma_1$, the proof of (i) follows directly from Lemma 2.2 and the proof of (ii) follows from Lemma 2.4 (i) as $n_3 = 1$.

(iii) On the contrary, assume that $m_{44} \geq 1$. Then there exists an edge $xy \in E(T)$ such that $d_T(x) = 4 = d_T(y)$. By using Lemma 2.4 (i) in (3), we obtain

$$\left.\begin{aligned} m_{13} + m_{14} &= 9, \\ m_{13} + 2\,m_{33} + m_{34} &= 3, \\ m_{14} + m_{34} + 2\,m_{44} &= 12. \end{aligned}\right\} \tag{5}$$

If $m_{13} = 0$, then from (5), we obtain $m_{14} = 9$, $m_{34} = 3$ and $m_{44} = 0$ as $m_{33} = 0$. Thus we get a contradiction as $m_{44} \geq 1$. Otherwise, $m_{13} \geq 1$. Then there exists an edge $uv \in E(T)$ such that $d_T(u) = 1$ and $d_T(v) = 3$. Without loss of generality, let x located on $u - y$ path in T. We obtain a tree T' from T as follows:

$$T' = T - xy - uv + vy + ux. \tag{6}$$

Then we see that $d_{T'}(t) = d_T(t)$ for all $t \in V(T)$ and

$$\mathcal{KD}_{\alpha,\beta}(T') - \mathcal{KD}_{\alpha,\beta}(T) = (1 + 4^\beta)^\alpha - (4^\beta + 4^\beta)^\alpha - (1 + 3^\beta)^\alpha + (4^\beta + 3^\beta)^\alpha.$$

By Lemma 2.1 (ii), we have

$$f_{1,4}(4) = (1 + 4^\beta)^\alpha - (4^\beta + 4^\beta)^\alpha > (1 + 3^\beta)^\alpha - (4^\beta + 3^\beta)^\alpha = f_{1,4}(3).$$

So $\mathcal{KD}_{\alpha,\beta}(T') > \mathcal{KD}_{\alpha,\beta}(T)$, which gives a contradiction. Hence $m_{44} = 0$.

(iv) By using Lemma 2.4 (i)–(iii) in (5), we obtain $m_{13} = 0$, $m_{14} = 9$ and $m_{34} = 3$. This completes the proof. □

LEMMA 2.5. *Let $T \in \Gamma_2$ be a chemical tree that maximizes $\mathcal{KD}_{\alpha,\beta}$ index for $\alpha \in (0, 1)$ and $\beta > 0$. Then* (i) $m_{44} = 0$, (ii) $m_{14} = 3n_4 = 3(n - 2b - 2)$, (iii) $m_{13} = 5b - 2n + 6$, $m_{34} = n_4 = n - 2b - 2$ *and* $m_{33} = 3b - n + 1$.

Proof. (i) On the contrary, assume that $m_{44} \geq 1$. Then T contains an edge $xy \in E(T)$ such that $d_T(x) = 4 = d_T(y)$.

Claim 2.6. At least one of m_{13} or m_{33} is nonzero.

Proof of Claim 2.6. By contradiction, we prove this result. For this, we assume that $m_{13} = 0 = m_{33}$. Setting $i = 1$ and $i = 3$ in (3), by Corollary 2.3, we obtain $m_{14} = n_1$ and $m_{34} = 3n_3$ as $m_{12} = m_{13} = m_{23} = m_{33} = 0$. Using these results and again Corollary 2.3 in (3) with setting $i = 4$, we obtain $m_{44} = 3n - 8b - 7$ as the degree sequence of T is $\pi_1(T)$. Since $T \in \Gamma_2$, we have $n \leq \lfloor \frac{5b+5}{2} \rfloor$ and hence $m_{44} \leq \frac{1-b}{2} < 0$, a contradiction as $m_{44} \geq 1$. This proves Claim 2.6. □

Now we further discuss the next two cases.

Case 1. If $m_{13} \neq 0$, then T possesses an edge $uv \in E(T)$ such that $d_T(u) = 1$ and $d_T(v) = 3$. Without loss of generality, suppose x lies on $u - y$ path in T. Using the transformation (6) and calculations in Lemma 2.4 (iii), one can easily get a contradiction. Thus we have $m_{44} = 0$.

Case 2. If $m_{33} \neq 0$, then T contains an edge $uv \in E(T)$ such that $d_T(u) = 3 = d_T(v)$. Without loss of generality, we assume that x and v lie on $u - y$ path in T. Using the transformation in (6), we obtain

$$\mathcal{KD}_{\alpha,\beta}(T') - \mathcal{KD}_{\alpha,\beta}(T) = (4^\beta + 3^\beta)^\alpha - (3^\beta + 3^\beta)^\alpha + (4^\alpha + 3^\beta)^\alpha - (4^\beta + 4^\beta)^\alpha.$$

By Lemma 2.1 (i), we have

$$f_{4,3}(3) = (4^\beta + 3^\beta)^\alpha - (3^\beta + 3^\beta)^\alpha > (4^\beta + 4^\beta)^\alpha - (3^\beta + 4^\beta)^\alpha = f_{4,3}(4).$$

This implies that $\mathcal{KD}_{\alpha,\beta}(T') > \mathcal{KD}_{\alpha,\beta}(T)$, which is a contradiction. Hence $m_{44} = 0$.

(ii) By contradiction, we prove that $3n_4 \leq m_{14}$. For this, we assume that $m_{14} < 3n_4$. This implies that T posesses a vertex w of degree 4 with at least two non-pendent neighbors, say w_1 and w_2. From Lemma 2.2, it is clear that $3 \leq d_T(w_1), d_T(w_2) \leq 4$. If $m_{13} = 0$, then $m_{14} = n_1$ (as $n_2 = 0$), and using the degree sequence in (4), we obtain $n - b = m_{14} < 3n_4 = 3\,(n - 2b - 2)$, that is, $n > \frac{5b+6}{2}$, yields a contradiction, as $T \in \Gamma_2$ (namely, $n \leq \lfloor \frac{5b+5}{2} \rfloor$). Otherwise, $m_{13} \neq 0$. Therefore, T possesses an edge $uv \in E(T)$ such that $d_T(u) = 3$ and $d_T(v) = 1$. Without loss of generality, let w_2 lies on $w-u$ path (w_2 may coincide with u). Now we obtain a tree T' as follows: $T' = T - ww_1 - uv + wv + uw_1$. This implies $d_{T'}(t) = d_T(t)$ for all $t \in V(T)$. Then

$$\begin{aligned}\mathcal{KD}_{\alpha,\,\beta}(T') - \mathcal{KD}_{\alpha,\,\beta}(T) = (4^\beta + 1)^\alpha - (3^\beta + 1)^\alpha + \big(3^\beta + d_T(w_1)^\beta\big)^\alpha \\ - \big(4^\beta + d_T(w_1)^\beta\big)^\alpha.\end{aligned}$$

By using Lemma 2.1 (ii), we obtain

$$\mathcal{KD}_{\alpha,\,\beta}(T') - \mathcal{KD}_{\alpha,\,\beta}(T) \geq (4^\beta + 1)^\alpha - (3^\beta + 1)^\alpha + (3^\beta + 3^\beta)^\alpha - (4^\beta + 3^\beta)^\alpha.$$

By Lemma 2.1 (i), we obtain

$$f_{4,3}(1) = (4^\beta + 1)^\alpha - (3^\beta + 1)^\alpha > (4^\beta + 3^\beta)^\alpha - (3^\beta + 3^\beta)^\alpha = f_{4,3}(3).$$

So $\mathcal{KD}_{\alpha,\beta}(T') > \mathcal{KD}_{\alpha,\beta}(T)$, which is a contradiction. Thus, we have $3n_4 \leq m_{14}$.

Since $T \in \Gamma_2$, we have $b \geq 2$, and hence any 4-degree vertex is adjacent to at most three pendant vertices in T. Thus, we have $3n_4 \geq m_{14}$. Consequently, $m_{14} = 3n_4$.

(iii) By using Lemmas 2.2, 2.5 (i) and (ii) and Corollary 2.3 in (3), we obtain

$$\left.\begin{aligned} m_{13} + 3\,(n - 2b - 2) &= n - b, \\ m_{13} + 2\,m_{33} + m_{34} &= 3\,(3b + 2 - n), \\ 3\,(n - 2b - 2) + m_{34} &= 4\,(n - 2b - 2). \end{aligned}\right\}$$

By simple computation in the above equation, we obtain $m_{13} = 5b - 2n + 6$, $m_{34} = n_4 = n - 2b - 2$ and $m_{33} = 3b - n + 1$. This completes the proof. □

Lemma 2.7. *Let $T \in \Gamma_3$ be a chemical tree that maximizes the $\mathcal{KD}_{\alpha,\beta}$ index for $\alpha \in (0, 1)$ and $\beta > 0$. Then* (i) *$m_{13} = 0$,* (ii) *$m_{14} = n_1 = n - b$,* (iii) *$m_{44} = 0$,* (iv) *$m_{34} = 3n - 7b - 8$ and $m_{33} = 8b + 7 - 3n$.*

Proof. (i) On the contrary, assume that $m_{13} \geq 1$. Then T contains an edge $uv \in E(T)$ such that $d_T(v) = 1$ and $d_T(u) = 3$. Since $T \in \Gamma_3$, we have $b \geq 6$, and hence any 4-degree vertex is adjacent to at most three pendant vertices in T. Thus, we have $3n_4 \geq m_{14}$. By applying Corollary 2.3 to (3) with $i = 1$, we obtain $m_{13} + m_{14} = n - b$. If $m_{14} = 3n_4 = 3(n - 2b - 2)$ (as $n_4 = n - 2b - 2$ by (4)), then from the above equation, we obtain $m_{13} = 5b - 2n + 6$. Since

$T \in \Gamma_3$, it holds that $m_{13} \leq 5b - 2\lceil \frac{5b+6}{2} \rceil + 6 \leq 0$, which is a contradiction as $m_{13} \geq 1$. Otherwise, $m_{14} < 3n_4$. Again, since $T \in \Gamma_3$, we have $n \geq \lceil \frac{5b+6}{2} \rceil$ and hence $n_4 = n - 2b - 2 > 0$. Then there exists at least two non-pendent neighbors of $w(d_T(w) = 4)$, say, w_1 and w_2. From Lemma 2.2, it is clear that $3 \leq d_T(w_1), d_T(w_2) \leq 4$. Without loss of generality, let w_2 be located on $w - u$ path (w_2 and u may coincide). By using the same transformation and calculations in Lemma 2.5 (ii), one can easily get a contradiction. Thus, we have $m_{13} = 0$.

(ii) Setting $i = 1$ in (3), then by Corollary 2.3 and Lemma 2.7 (i), we obtain $m_{14} = n_1 = n - b$.

(iii) On the contrary, assume that $m_{44} \geq 1$. Then T possesses an edge $xy \in E(T)$ such that $d_T(x) = 4 = d_T(y)$. Setting $i = 3$ in (3) with Corollary 2.3 and Lemma 2.7 (i), we obtain $2m_{33} + m_{34} = 3(3b + 2 - n)$, by (4). If $m_{33} = 0$, then from the above equation, we obtain $m_{34} = 3(3b + 2 - n)$. Setting $i = 4$ in (3) with Corollary 2.3 and Lemma 2.7 (ii) and $m_{34} = 3(3b + 2 - n)$, we obtain $m_{44} = 3n - 8b - 7$. Since $T \in \Gamma_3$, it follows that $m_{44} \leq 3\lfloor \frac{8b+7}{3} \rfloor - 8b - 7 \leq 0$, a contradiction as $m_{44} \geq 1$. Otherwise, $m_{33} \geq 1$. Then T contains an edge $uv \in E(T)$ such that $d_T(u) = 3 = d_T(v)$. Without loss of generality, suppose that x and v lie on $u - y$ path. Using the same transformation and computations outlined in Case 2 of Lemma 2.5 (i), one can easily get a contradiction. Hence $m_{44} = 0$.

(iv) Using Corollary 2.3 and Lemma 2.7 (i)–(iii) in (3), we obtain

$$\left.\begin{aligned} m_{13} + m_{14} &= n - b, \\ m_{13} + 2\,m_{33} + m_{34} &= 3\,(3b + 2 - n), \\ n - b + m_{34} &= 4\,(n - 2b - 2). \end{aligned}\right\}$$

By solving simultaneously the above equations, we obtain $m_{34} = 3n - 7b - 8$ and $m_{33} = 8b + 7 - 3n$. This completes the proof. □

LEMMA 2.8. *Let $T \in \Gamma_4$ be a chemical tree that maximizes the $\mathcal{KD}_{\alpha,\beta}$ index for $\alpha \in (0, 1)$ and $\beta > 0$. Then* (i) *$m_{13} = 0$,* (ii) *$m_{14} = n - b$,* (iii) *$m_{33} = 0$,* (iv) *$m_{34} = 9b + 6 - 3n$ and $m_{44} = 3n - 8b - 7$.*

Proof. (i) By using similar arguments and transformation as given in Lemma 2.7 (i), one can easily obtain $m_{13} = 0$.

(ii) Choosing $i = 1$ in (3), then by Corollary 2.3 and Lemma 2.8 (i), we obtain $m_{14} = n_1 = n - b$.

(iii) On the contrary, assume that $m_{33} \geq 1$. Then T possesses an edge $uv \in E(T)$ such that $d_T(u) = 3 = d_T(v)$. Setting $i = 4$ in (3) with Lemmas 2.2, 2.8 (ii) and Corollary 2.3, we obtain $n - b + m_{34} + 2m_{44} = 4(n - 2b - 2)$.

Next, if $m_{44} = 0$, then we obtain $m_{34} = 3n - 7b - 8$. Setting $i = 3$ in (3) with Corollary 2.3 and Lemma 2.8 (i) (namely, $m_{23} = m_{13} = 0$) and $m_{34} = 3n - 7b - 8$, we obtain $m_{33} = 8b + 7 - 3n$. Since $T \in \Gamma_4$, we obtain $m_{33} \leq 8b + 7 - 3\lceil \frac{8b+8}{3} \rceil < 0$, a contradiction as $m_{33} \geq 1$. Otherwise, $m_{44} \geq 1$. Then T contains an edge $xy \in E(T)$ such that $d_T(x) = 4 = d_T(y)$. Without loss of generality, let x and v lie on $u - y$ path. Using the same transformation and calculations as in Case 2 of Lemma 2.5 (i), one can easily get a contradiction. Hence $m_{33} = 0$.

(iv) Setting $i = 3$ and $i = 4$ in (3) with Lemmas 2.2, 2.8 (i)–(iii) and Corollary 2.3, we obtain

$$\left.\begin{aligned} m_{34} &= 3(3b + 2 - n), \\ n - b + 9b + 6 - 3n + 2m_{44} &= 4(n - 2b - 2). \end{aligned}\right\}$$

From the above equation, we obtain $m_{34} = 9b + 6 - 3n$ and $m_{44} = 3n - 8b - 7$. This completes the proof. □

We define the degree sequence $\pi_2(T)$ as follows:

$$\pi_2(T) = (\underbrace{4, \ldots, 4}_{b}, \underbrace{2, \ldots, 2}_{n-3b-2}, \underbrace{1, \ldots, 1}_{2(b+1)}). \tag{7}$$

Lemma 2.9. *Let $T \in \mathcal{CT}''_{n,b}\,(n \geq 6)$ be a chemical tree that maximizes the $\mathcal{KD}_{\alpha,\beta}$ index for $\alpha \in (0, 1]$ and $\beta > 0$. Then T has the degree sequence $\pi_2(T)$ defined in (7).*

Proof. On the contrary, assume that $n_3 \geq 1$. Then there exists $x \in V(T)$ with $d_T(x) = 3$. Let $N_T(x) = \{x_1, x_2, x_3\}$. Since $T \in \mathcal{CT}''_{n,b}$, we have $n \geq 3b + 3$. If $n_2 = 0$, then from (1) and (2), we obtain $n = 2 + 2b + n_4$ as $n_3 + n_4 = b$. Since $n_4 \leq b$, we obtain $n \leq 3b + 2$, which is a contradiction as $n \geq 3b + 3$. Otherwise, $n_2 \geq 1$. Then T possesses a vertex $w \in V(T)$ such that $d_T(w) = 2$. Using the same technique described in Lemma 2.2, one can easily get a contradiction. Hence $n_3 = 0$.

Using $n_3 = 0$ in (1) and (2) and solving them simultaneously, we obtain the degree sequence

$$\pi_2(T) = (\underbrace{4, \ldots, 4}_{b}, \underbrace{2, \ldots, 2}_{n-3b-2}, \underbrace{1, \ldots, 1}_{2b+2}) \text{ as } n_4 = b.$$

This completes the proof. □

The following corollary is a direct consequence of Lemma 2.9.

Corollary 2.10. *Let $T \in \mathcal{CT}''_{n,b}\,(n \geq 6)$ be a chemical tree that maximizes the $\mathcal{KD}_{\alpha,\beta}$ index for $\alpha \in (0, 1]$ and $\beta > 0$. Then $n_3 = 0$, that is, $m_{13} = m_{23} = m_{33} = m_{34} = 0$.*

LEMMA 2.11. *Let $T \in \Gamma_5$ be a chemical tree that maximizes the $\mathcal{KD}_{\alpha,\beta}$ index for $\alpha \in (0,1)$ and $\beta > 0$. Then* (i) $n_1 = 4$, $n_2 = n-5$, $n_4 = 1$, $m_{44} = 0$, (ii) $m_{14} = 3$, (iii) $m_{22} = n-6$, $m_{12} = 1$ *and* $m_{24} = 1$.

Proof. Since $T \in \Gamma_5$, we have $T \in \mathcal{CT}''_{n,b}$ and $b = 1$. By Lemma 2.9, the degree sequence of T ($\pi_2(T)$) is defined in (7). Since $b = 1$, we have $n_1 = 4$, $n_2 = n-5$, $n_4 = 1$, $m_{44} = 0$. This proves the result of (i).

(ii) Since $T \in \Gamma_5$, we have $b = 1$, $n \geq 6$, and hence a 4-degree vertex is adjacent to at most three pendant vertices in T. Thus, we have $m_{14} \leq 3$. By contradiction, we prove that $m_{14} = 3$. For this, we assume that $m_{14} < 3$. Then there exists a vertex $w \in V(T)$ of degree 4 with at least two non-pendent neighbors, say w_1 and w_2. Let $x \notin N_T(w)$ be a pendent vertex, and x_1 be its neighbor. Without loss of generality, suppose w_2 lies on $w - x$ path (w_2 may coincide with x_1). Since $T \in \Gamma_5$ ($b = 1$), it is obvious that $d_T(w_1) = 2 = d_T(w_2)$ and $d_T(x_1) = 2$. We construct a tree T' from T as follows: $T' = T - ww_1 - xx_1 + wx + x_1w_1$. This gives $d_{T'}(t) = d_T(t)$ for all $t \in V(T)$. Then

$$\mathcal{KD}_{\alpha,\beta}(T') - \mathcal{KD}_{\alpha,\beta}(T) = (4^\beta + 1)^\alpha + (2^\beta + 2^\beta)^\alpha - (4^\beta + 2^\beta)^\alpha - (2^\beta + 1)^\alpha.$$

By Lemma 2.1 (ii), we obtain

$$f_{1,2}(4) = (1 + 4^\beta)^\alpha - (2^\beta + 4^\beta)^\alpha > (1 + 2^\beta)^\alpha - (2^\beta + 2^\beta)^\alpha = f_{1,2}(2).$$

This implies $\mathcal{KD}_{\alpha,\beta}(T') > \mathcal{KD}_{\alpha,\beta}(T)$, which is a contradiction. Thus, we have $m_{14} = 3$.

(iii) By using Corollary 2.10 and Lemma 2.11 (i) and (ii) in (3), we obtain

$$\left.\begin{aligned} m_{12} + 3 &= 4, \\ m_{12} + 2\,m_{22} + m_{24} &= 2\,(n-5), \\ 3 + m_{24} &= 4. \end{aligned}\right\}$$

From the above equation, we obtain $m_{22} = n-6$, $m_{12} = 1$ and $m_{24} = 1$. This completes the proof. □

LEMMA 2.12. *Let $T \in \Gamma_6$ be a chemical tree that maximizes the $\mathcal{KD}_{\alpha,\beta}$ index for $\alpha \in (0,1)$ and $\beta > 0$. Then* (i) $m_{12} = 0$, (ii) $m_{14} = 2b + 2$, (iii) $m_{22} = 0$, (iv) $m_{44} = 4b + 1 - n$ *and* $m_{24} = 2n - 6b - 4$.

Proof. (i) On the contrary, assume that $m_{12} \geq 1$. Then there exists an edge $xx_1 \in E(T)$ such that $d_T(x_1) = 2$ and $d_T(x) = 1$. Since $T \in \Gamma_6$, we have $b \geq 2$ and there exist $v, w \in V(T)$ such that $d_T(w) = 4 = d_T(v)$, by Lemma 2.9. Without loss of generality, let w lies on the $x - v$ path. Now we discuss the proof in two cases.

Case 1. $vw \in E(T)$. Construct a tree T' from T as

$$T' = T - xx_1 - vw + vx_1 + wx.$$

Then we see that $d_{T'}(t) = d_T(t)$ for all $t \in V(T)$. Therefore

$$\mathcal{KD}_{\alpha,\beta}(T') - \mathcal{KD}_{\alpha,\beta}(T) = (2^\beta + 4^\beta)^\alpha + (4^\beta + 1)^\alpha - (2^\beta + 1)^\alpha - (4^\beta + 4^\beta)^\alpha.$$

By Lemma 2.1 (i), we obtain

$$f_{4,2}(1) = (4^\beta + 1)^\alpha - (2^\beta + 1)^\alpha > (4^\beta + 4^\beta)^\alpha - (2^\beta + 4^\beta)^\alpha = f_{4,2}(4).$$

This shows $\mathcal{KD}_{\alpha,\beta}(T') > \mathcal{KD}_{\alpha,\beta}(T)$, which is a contradiction. Thus, we have $m_{12} = 0$.

Case 2. $vw \notin E(T)$. Let $P_{wv} = ww_1 \cdots w_s v$ be a shortest $w - v$ path. From Lemma 2.9, it is clear that $d_T(w_j) = 2$, for all j, $1 \le j \le s$. We construct a tree T' from T as $T' = T - ww_1 - xx_1 + wx + x_1w_1$. This gives $d_{T'}(t) = d_T(t)$ for all $t \in V(T)$. Using the same calculation as in Lemma 2.11 (ii), one can easily get a contradiction. Thus we obtain $m_{12} = 0$.

(ii) Setting $i = 1$ in (3) with $m_{13} = 0 = m_{12}$, we obtain $m_{14} = n_1 = 2b+2$, by (7).

(iii) On the contrary, assume that $m_{22} \ge 1$. Then there exists an edge $xy \in E(T)$ such that $d_T(x) = 2 = d_T(y)$. Setting $i = 4$ in (3) with Lemmas 2.9, 2.12 (ii) and Corollary 2.10, we get $2b + 2 + m_{24} + 2m_{44} = 4n_4 = 4b$, that is, $m_{24} + 2m_{44} = 2\,(b - 1)$. First, we assume that $m_{44} = 0$. Then by the above equation, we obtain $m_{24} = 2b - 2$. Choosing $i = 2$ in (3) with $m_{23} = 0 = m_{12}$ and $m_{24} = 2b - 2$, we obtain $2b - 2 + 2m_{22} = 2n_2 = 2(n - 3b - 2)$, that is, $m_{22} = n - 4b - 1$. Since $T \in \Gamma_6$, we have $n \le 4b + 1$ and hence $m_{22} \le 0$, which is a contradiction as $m_{22} \ge 1$.

Next, we assume that $m_{44} \ge 1$. Then there exists an edge $uv \in E(T)$ such that $d_T(u) = 4 = d_T(v)$. Without loss of generality, we suppose that x and v lie on the $y - u$ path. Now we construct a tree T' from T as $T' = T - uv - xy + ux + yv$. Then $d_{T'}(t) = d_T(t)$ for all $t \in V(T)$. Therefore

$$\mathcal{KD}_{\alpha,\beta}(T') - \mathcal{KD}_{\alpha,\beta}(T) = (4^\beta + 2^\beta)^\alpha + (4^\beta + 2^\beta)^\alpha - (2^\beta + 2^\beta)^\alpha - (4^\beta + 4^\beta)^\alpha.$$

By Lemma 2.1 (i), we obtain

$$f_{4,2}(2) = (4^\beta + 2^\beta)^\alpha - (2^\beta + 2^\beta)^\alpha > (4^\beta + 4^\beta)^\alpha - (2^\beta + 4^\beta)^\alpha = f_{4,2}(4).$$

This gives $\mathcal{KD}_{\alpha,\beta}(T') > \mathcal{KD}_{\alpha,\beta}(T)$, which is a contradiction. Consequently, $m_{22} = 0$.

(iv) Setting $i = 2$ and $i = 4$ in (3) with Corollary 2.10 and Lemmas 2.12 (i)–(iii), we obtain

$$\left.\begin{aligned} m_{24} &= 2\,(n - 3b - 2), \\ 2b + 2 + m_{24} + 2m_{44} &= 4b. \end{aligned}\right\}$$

From the above equations, we obtain $m_{44} = 4b+1-n$ and $m_{24} = 2n-6b-4$. This completes the proof. □

Lemma 2.13. *Let $T \in \Gamma_7$ be a chemical tree that maximizes the $\mathcal{KD}_{\alpha,\beta}$ index for $\alpha \in (0,1)$ and $\beta > 0$. Then* (i) $m_{12} = 0$, (ii) $m_{14} = 2b+2$, (iii) $m_{44} = 0$, (iv) $m_{22} = n-4b-1$ *and* $m_{24} = 2b-2$.

Proof. The proofs of (i) and (ii) are analogous to Lemma 2.12 (i) and (ii), respectively.

(iii) On the contrary, assume that $m_{44} \geq 1$. Then T possesses an edge $uv \in E(T)$ such that $d_T(u) = 4 = d_T(v)$. Setting $i = 2$ in (3) with Corollary 2.10 and Lemma 2.13 (i) ($m_{23} = 0 = m_{12}$), we get $2m_{22} + m_{24} = 2n_2 = 2(n-3b-2)$. If $m_{22} = 0$, then from this equation, we get $m_{24} = 2n-6b-4$. Now choosing $i = 4$ in (3) with $m_{24} = 2n-6b-4$ and Lemmas 2.9, 2.13 (ii) and Corollary 2.10, we obtain $2n-6b-4+2b+2+2m_{44} = 4b$, that is, $m_{44} = 4b+1-n$. Since $T \in \Gamma_7$, we have $n \geq 4b+2$ and hence $m_{44} < 0$, which is a contradiction. Otherwise, $m_{22} \geq 1$. Then T contains an edge $xy \in E(T)$ such that $d_T(x) = 2 = d_T(y)$. Without loss of generality, let x and v are on the path $y-u$. Using the same transformation and calculations as in Lemma 2.12 (iii), one easily gets a contradiction. Thus, we have $m_{44} = 0$.

(iv) Choosing $i = 2$ and $i = 4$ in (3) with Corollary 2.10 and Lemma 2.13 (i)–(iii), we obtain

$$\left.\begin{aligned} 2m_{22} + m_{24} &= 2\,(n-3b-2), \\ 2b+2+m_{24} &= 4b. \end{aligned}\right\}$$

From the above equations, we obtain $m_{22} = n-4b-1$, and $m_{24} = 2b-2$. This completes the proof. □

The first Zagreb index ($\mathcal{M}_1(G) = \sum_{x\in V(G)} d_G^2(x)$) and forgotten index ($\mathcal{F}(G) = \sum_{x\in V(G)} d_G^3(x)$) can be obtained from $\mathcal{KD}_{\alpha,\beta}$ when $\alpha = 1 = \beta$, and $\alpha = 1$ and $\beta = 2$, respectively. Thus from Lemmas 2.2 and 2.9, we have the following result.

Theorem 2.14. *Let $T \in \mathcal{CT}_{n,b}$ be a chemical tree with $n \geq 6$. Then*

$$\mathcal{M}_1(T) \leq \begin{cases} 4n+6b-6 & \text{if } 2(b+1) \leq n \leq 3b+2 \text{ and } b \geq 2, \\ 8n-6b-14 & \text{if } n \geq 3b+3 \text{ and } b \geq 1, \end{cases}$$

$$\mathcal{F}(T) \leq \begin{cases} 38n-48b-74 & \text{if } 2(b+1) \leq n \leq 3b+2 \text{ and } b \geq 2, \\ 42n+8n-14 & \text{if } n \geq 3b+3 \text{ and } b \geq 1. \end{cases}$$

The equality holds in $\mathcal{M}_1(T) \leq 4n+6b-6$ (or $\mathcal{F}(T) \leq 38n-48b-74$) for $2b+2 \leq n \leq 3b+2$ and $b \geq 2$ if and only if T has the degree sequence π_1.

Similarly, the inequality $\mathcal{M}_1(T) \leq 8n-6b-14$ (or $\mathcal{F}(T) \leq 42n+8n-14$) turns into equality for $n \geq 3b+3$ and $b \geq 1$ if and only if T has degree sequence π_2.

If $n = 4$ and $b = 1$, then $\mathcal{CT}_{4,1} = \{S_4\}$. Thus $\mathcal{KD}_{\alpha,\beta}(S_4) = 3(3^\beta + 1)^\alpha$. From Lemma 2.2, $\mathcal{CT}_{n,b}$ has only one tree, that is, S_5 when $n = 5$ and $b = 1$. Thus we obtain $\mathcal{KD}_{\alpha,\beta}(S_5) = 4(4^\beta + 1)^\alpha$.

Let $\mathcal{C}_1\mathcal{T}_{n,b}$ denotes the subclass of chemical trees in $\mathcal{CT}'_{n,b}$ for $n \geq 6$ and $b \geq 1$ with degree sequences

$$\pi_1 = (\underbrace{4,\ldots,4}_{n-2b-2},\underbrace{3,\ldots,3}_{3b+2-n},\underbrace{1,\ldots,1}_{n-b})$$

and defined as follows:

$$\mathcal{C}_1\mathcal{T}_{n,b} = \Gamma_1' \cup \Gamma_2' \cup \Gamma_3' \cup \Gamma_4',$$

where

$$\Gamma_1' = \{T \in \Gamma_1 : n_2 = 0, m_{33} = m_{44} = m_{13} = 0, m_{14} = 9, m_{34} = 3\},$$
$$\Gamma_2' = \{T \in \Gamma_2 : n_2 = 0, m_{44} = 0, m_{14} = 3n-6b-6, m_{13} = 5b-2n+6, m_{34} = n-2b-2, m_{33} = 3b-n+1\},$$
$$\Gamma_3' = \{T \in \Gamma_2 : n_2 = 0, m_{44} = m_{13} = 0, m_{14} = n-b, m_{33} = 8b+7-3n, m_{34} = 3n-7b-8\},$$
$$\Gamma_4' = \{T \in \Gamma_4 : n_2 = 0, m_{33} = m_{13} = 0, m_{14} = n-b, m_{44} = 3n-8b-7, m_{34} = 9b+6-3n\}.$$

Let $\mathcal{C}_2\mathcal{T}_{n,b} \subseteq \mathcal{CT}''_{n,b}$ denotes the subclass of chemical trees for $n \geq 6$ and $b \geq 1$ with degree sequences

$$\pi_2 = (\underbrace{4,\ldots,4}_{b},\underbrace{2,\ldots,2}_{n-3b-2},\underbrace{1,\ldots,1}_{2b+2}),$$

and defined as follows:

$$\mathcal{C}_2\mathcal{T}_{n,b} = \Gamma_5' \cup \Gamma_6' \cup \Gamma_7',$$

where

$$\Gamma_5' = \{T \in \Gamma_5 : n_3 = 0, m_{14} = 3, m_{12} = 1, m_{22} = n-6, m_{24} = 1\},$$
$$\Gamma_6' = \{T \in \Gamma_2 : n_3 = 0, m_{12} = m_{22} = 0, m_{14} = 2b+2, m_{44} = 4b+1-n, m_{24} = 2n-6b-4\},$$
$$\Gamma_7' = \{T \in \Gamma_2 : n_3 = 0, m_{12} = m_{44} = 0, m_{14} = 2b+2, m_{22} = n-4b-1, m_{24} = 2b-2\}.$$

To visualize the chemical trees in $\mathcal{C}_1\mathcal{T}_{n,b}$, refer to $T_2 \in \Gamma_1'$; $T_4, T_5 \in \Gamma_2'$; $T_7, T_8 \in \Gamma_3'$; and $T_{10}, T_{11} \in \Gamma_4'$ as illustrated in Figure 1. Similarly, for the chemical trees in $\mathcal{C}_2\mathcal{T}_{n,b}$, see $T_{13} \in \Gamma_5'$; $T_{16}, T_{17} \in \Gamma_6'$; and $T_{19}, T_{20} \in \Gamma_7'$ in Figure 1.

Based on Lemmas 2.2–2.13 and Corollaries 2.3 and 2.10, the structural configuration of a chemical tree that achieves the optimal upper bound for the $\mathcal{KD}_{\alpha,\beta}$ index has been completely characterized, allowing us to state the following theorem.

THEOREM 2.15. *Let $T \in \mathcal{CT}_{n,b}$ be a chemical tree. If $\alpha \in (0,1)$ and $\beta > 0$, then*

$$\mathcal{KD}_{\alpha,\beta}(T) \leq \begin{cases} 9(1+4^{\beta})^{\alpha}+3(3^{\beta}+4^{\beta})^{\alpha} & \text{if } n=13 \text{ and } b=4,\\ 3(n-2b-2)(1+4^{\beta})^{\alpha}+(5b-2n+6)(1+3^{\beta})^{\alpha}+(n-2b-2)(3^{\beta}+4^{\beta})^{\alpha} & \\ \quad +(3b-n+1)(2\cdot 3^{\beta})^{\alpha} & \text{if } 2b+2 \leq n \leq \lfloor \frac{5b+5}{2} \rfloor \text{ and } b \geq 2,\\ (n-b)(1+4^{\beta})^{\alpha}+(3n-7b-8)(3^{\beta}+4^{\beta})^{\alpha}+(8b-3n+7)(2\cdot 3^{\beta})^{\alpha} & \\ & \text{if } \lceil \frac{5b+6}{2} \rceil \leq n \leq \lfloor \frac{8b+7}{3} \rfloor \text{ and } b \geq 6,\\ (n-b)(1+4^{\beta})^{\alpha}+3\,(3b+2-n)(3^{\beta}+4^{\beta})^{\alpha}+(3n-8b-7)\,2^{(2\beta+1)\alpha} & \\ & \text{if } \lceil \frac{8b+8}{3} \rceil \leq n \leq 3b+2 \text{ and } b \geq 2,\\ 3(1+4^{\beta})^{\alpha}+(n-6)2^{(\beta+1)\alpha}+(1+2^{\beta})^{\alpha}+2^{\alpha\beta}(1+2^{\beta})^{\alpha} & \\ & \text{if } n \geq 3b+3 \text{ and } b=1,\\ 2(b+1)(1+4^{\beta})^{\alpha}+(4b+1-n)2^{(2\beta+1)\alpha}+(n-3b-2)2^{\alpha\beta+1}(1+2^{\beta})^{\alpha} & \\ & \text{if } 3b+3 \leq n \leq 4b+1 \text{ and } b \geq 2,\\ 2(b+1)(1+4^{\beta})^{\alpha}+(n-4b-1)2^{\alpha(\beta+1)}+(b-1)\,2^{\alpha\beta+1}\,(1+2^{\beta})^{\alpha} & \\ & \text{if } n \geq 4b+2 \text{ and } b \geq 2. \end{cases}$$

The equality holds if and only if $T \in \mathcal{C}_1\mathcal{T}_{n,b}$ for $2b+2 \leq n \leq 3b+2 (b \geq 2)$, and $n = 13$ and $b = 4$. The equality attains if and only if $T \in \mathcal{C}_2\mathcal{T}_{n,b}$ for $n \geq 3b+3$ and $b \geq 1$.

Proof. Let $T^{\star}$ be a chemical tree with the highest value of $\mathcal{KD}_{\alpha,\,\beta}$ index with $\alpha \in (0,1)$ and $\beta > 0$ in $\mathcal{CT}_{n,b}\,(b \geq 1)$. Since

$$\mathcal{CT}_{n,b} = \mathcal{CT}'_{n,b} \cup \mathcal{CT}''_{n,b} = (\Gamma_1 \cup \Gamma_2 \cup \Gamma_3 \cup \Gamma_4) \cup (\Gamma_5 \cup \Gamma_6 \cup \Gamma_7),$$

therefore, we discuss the proof in two cases.

Case 1. $T^{\star} \in \mathcal{CT}'_{n,b} = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3 \cup \Gamma_4$. By Lemma 2.2, the chemical tree $T^{\star}$ has degree sequence

$$(\underbrace{4,\cdots,4}_{n-2(b+1)},\underbrace{3,\ldots,3}_{3b+2-n},\underbrace{1,\ldots,1}_{n-b}),$$

and hence by Corollary 2.3, we have $n_2 = 0$, that is, $m_{2i} = 0$ for all $i \in \{1,2,3,4\}$. Now, on the basis of Lemmas 2.4–2.8, we discuss the further following cases:

Case 1.1. $T^\star \in \Gamma_1$. By Lemma 2.4 (ii)–(iv), we obtain $m_{33} = m_{44} = m_{13} = 0, m_{14} = 9$ and $m_{34} = 3$. Since $n_2 = 0$, we conclude that $T^\star \in \Gamma_1'$, and hence

$$\mathcal{KD}_{\alpha,\beta}(T^\star) = 9\,(1+4^\beta)^\alpha + 3\,(3^\beta+4^\beta)^\alpha.$$

Case 1.2. $T^\star \in \Gamma_2$. By Lemma 2.5, we acquire $m_{44} = 0$, $m_{14} = 3n_4 = 3n-6b-6$, $m_{13} = 5b-2n+6$, $m_{34} = n_4 = n-2b-2$ and $m_{33} = 3b-n+1$. Since $n_2 = 0$, therefore $T^\star \in \Gamma_2'$. Consequently,

$$\begin{aligned}\mathcal{KD}_{\alpha,\beta}(T^\star) &= 3(n-2b-2)(1+4^\beta)^\alpha + (5b-2n+6)(1+3^\beta)^\alpha \\ &\quad + (n-2b-2)(3^\beta+4^\beta)^\alpha + (3b-n+1)(2\cdot 3^\beta)^\alpha.\end{aligned}$$

Case 1.3. $T^\star \in \Gamma_3$. From Lemma 2.7, we obtain $m_{13} = 0 = m_{44}$, $m_{14} = n-b$, $m_{34} = 3n-7b-8$ and $m_{33} = 8b-3n+7$. Since $n_2 = 0$, thus $T^\star \in \Gamma_3'$, and hence

$$\begin{aligned}\mathcal{KD}_{\alpha,\beta}(T^\star) &= (n-b)(1+4^\beta)^\alpha + (3n-7b-8)(3^\beta+4^\beta)^\alpha \\ &\quad + (8b-3n+7)(2\cdot 3^\beta)^\alpha.\end{aligned}$$

Case 1.4. $T^\star \in \Gamma_4$. Using Lemma 2.8, we acquire $m_{13} = 0 = m_{33}$, $m_{14} = n-b$, $m_{34} = 9b+6-3n$ and $m_{44} = 3n-8b-7$. Since $n_2 = 0$, so $T^\star \in \Gamma_4'$. Consequently

$$\begin{aligned}\mathcal{KD}_{\alpha,\beta}(T^\star) &= (n-b)(1+4^\beta)^\alpha + 3\,(3b+2-n)(3^\beta+4^\beta)^\alpha \\ &\quad + (3n-8b-7)\,2^{(2\beta+1)\alpha}.\end{aligned}$$

From the above cases, it holds that $T^\star \in \mathcal{C}_1\mathcal{T}_{n,b} = \Gamma_1' \cup \Gamma_2' \cup \Gamma_3' \cup \Gamma_4'$.

Case 2. $T^\star \in \mathcal{CT}''_{n,b} = \Gamma_5 \cup \Gamma_6 \cup \Gamma_7$. By Lemma 2.9, the chemical tree $T^\star \in \mathcal{CT}''_{n,b}$ has degree sequence

$$(\underbrace{4,\ldots,4}_{b}, \underbrace{2,\ldots,2}_{n-3b-2}, \underbrace{1,\ldots,1}_{2b+2}),$$

and so by Corollary 2.10, we have $n_3 = 0$, that is, $m_{i3} = 0$ for all $i = \{1,2,3,4\}$. Now by Lemmas 2.11–2.13, the further following cases arise.

Case 2.1. $T^\star \in \Gamma_5$. By Lemma 2.11, we obtain $m_{44} = 0$, $m_{14} = 3$, $m_{22} = n-6$ and $m_{12} = 1 = m_{24}$. Since $n_3 = 0$, we conclude that $T^\star \in \Gamma_5'$, and hence

$$\mathcal{KD}_{\alpha,\beta}(T^\star) = 3\,(1+4^\beta)^\alpha + (n-6)\,2^{(\beta+1)\alpha} + (1+2^\beta)^\alpha + 2^{\alpha\beta}\,(1+2^\beta)^\alpha.$$

Case 2.2. $T^\star \in \Gamma_6$. Using Lemma 2.12, we acquire $m_{12} = m_{22} = 0$, $m_{14} = 2b+2$, $m_{44} = 4b+1-n$ and $m_{24} = 2n-6b-4$. Since $n_3 = 0$, consequently $T^\star \in \Gamma_6'$. As a result

$$\mathcal{KD}_{\alpha,\beta}(T^\star) = 2(b+1)(1+4^\beta)^\alpha + (4b+1-n)2^{(2\beta+1)\alpha}$$

$$+ (n-3b-2)2^{\alpha\beta+1}(1+2^{\beta})^{\alpha}.$$

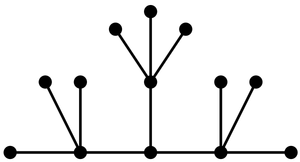
Case 2.3. $T^{\star} \in \Gamma_7$. Using Lemma 2.13, we have $m_{12} = m_{44} = 0$, $m_{14} = 2b+2$, $m_{22} = n-4b-1$ and $m_{24} = 2b-2$. Since $n_3 = 0$, this implies $T^{\star} \in \Gamma_7'$, and hence

$$\mathcal{KD}_{\alpha,\beta}(T^{\star}) = 2(b+1)(1+4^{\beta})^{\alpha} + (n-4b-1)2^{\alpha(\beta+1)} + (b-1)2^{\alpha\beta+1}(1+2^{\beta})^{\alpha}.$$

Hence, from the above cases, it follows that $T^{\star} \in \mathcal{C}_2\mathcal{T}_{n,b} = \Gamma_5' \cup \Gamma_6' \cup \Gamma_7'$. This completes the proof of this theorem. □

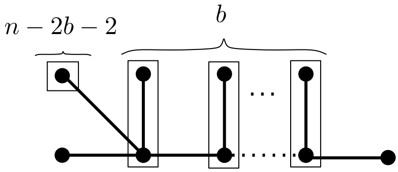
Remark 2.16. When $\beta = 2$, we have $\mathcal{KD}_{\alpha,2} = \mathcal{SO}_{\alpha}$. Thus, Theorem 2.15 also holds for the general Sombor index. Since $\alpha \in (0,1)$ in Theorem 2.15, this implies that $\mathcal{SO}_{1/2} = \mathcal{SO}$. Thus, the results also hold for the Sombor index. In particular, the $\mathcal{SO}_{\alpha}$ index generalizes the result in [3] (see Theorems 1–5).

Remark 2.17. When $\beta = 1$, we have $\mathcal{KD}_{\alpha,1} = \mathcal{X}_{\alpha}$. Therefore, Theorem 2.15 also holds for the general sum-connectivity index. Since $\alpha \in (0,1)$ in Theorem 2.15, this implies that $\mathcal{X}_{1/2} = \mathcal{N}$. Thus, the results also hold for the Nirmala index. Notably, $\mathcal{X}_{\alpha}$ generalizes the result of first Zagreb index, see Theorem 2.14 and also Theorem 3 in [28].



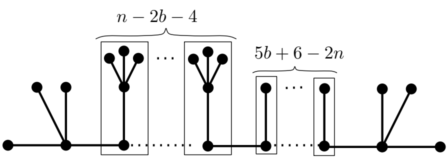
T_{22}

Figure 2 – $T_{22} \in \Gamma_1'$.



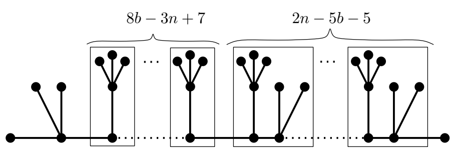
T_{23}

Figure 3 – $T_{23} \in \Gamma_2'$, $2b+2 \le n \le 2b+3$, $b \ge 2$.



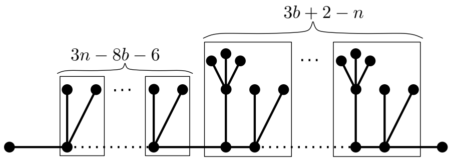
T_{24}

Figure 4 – $T_{24} \in \Gamma_2'$, $2b+4 \le n \le \lfloor \frac{5b+5}{2} \rfloor$, $b \ge 2$.



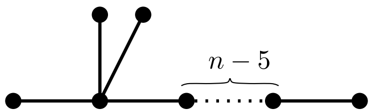
T_{25}

Figure 5 – $T_{25} \in \Gamma_3'$.



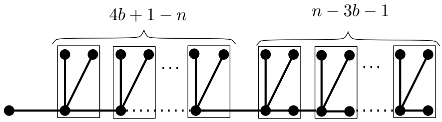
T_{26}

Figure 6 – $T_{26} \in \Gamma'_4$.



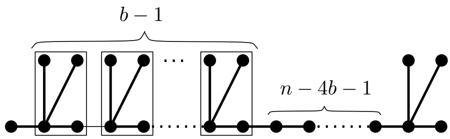
T_{27}

Figure 7 – $T_{27} \in \Gamma'_5$.



T_{28}

Figure 8 – $T_{28} \in \Gamma'_6$.



T_{29}

Figure 9 – $T_{29} \in \Gamma'_7$.

2.1. Construction of maximal chemical trees in $\mathcal{CT}_{n,b}$

In this subsection, we present the construction of maximal chemical trees in $\mathcal{CT}_{n,b}$ with respect to the $\mathcal{KD}_{\alpha,\beta}$ index, where $\alpha \in (0,1)$ and $\beta > 0$. The constructions provided are generalized forms that, by fixing the values of n and b, allow for the derivation of the corresponding maximal chemical trees, which establish the upper bound. For instance, see Figures 2–9. Specifically, in Figure 2, for $b = 4$ and $n = 13$, T_{22} is the unique maximal tree in Γ'_1. Additionally, for $b \geq 2$ and $2b+2 \leq n \leq 2b+3$, each chemical tree in Figure 3 belongs to Γ'_2. Similarly, each chemical tree in Figure 4 also belongs to Γ'_2, and by assigning specific values of given n and b, the resulting chemical tree satisfies the structural properties of Γ'_2. Likewise, the chemical trees generated in Figure 5, with appropriate values, belong to Γ'_3, the trees in Figure 6 belong to Γ'_4, the trees in Figure 7 belong to Γ'_5, the trees in Figure 8 belong to Γ'_6 and the trees in Figure 9 belong to Γ'_7.

3. CONCLUDING REMARKS

In this paper, we successfully characterized the chemical trees in $\mathcal{CT}_{n,b}$ with respect to the $\mathcal{KD}_{\alpha,\beta}$ index for $\alpha \in (0,1]$ and $\beta > 0$. Notably, Theorem 2.15 encompasses the traditional general Sombor index, as $\mathcal{KD}_{\alpha,2} = \mathcal{SO}_\alpha$, thereby generalizing the results of the Sombor index in [3]. In addition, since

$\mathcal{SO}_1 = \mathcal{F}$, our findings extend to the forgotten index as well. Similarly, Theorem 2.15 covers the general sum-connectivity index, as $\mathcal{KD}_{\alpha,1} = \mathcal{X}_\alpha$, and generalizes the first Zagreb index problem in [28].

We explore the general Platt index [25], defined for a graph G as:

$$Pl_\alpha(G) = \sum_{xy \in E(G)} \big(d_G(x) + d_G(y) - 2\big)^\alpha,$$

where α is a nonzero real number. Since the structure of Pl_α is similar to $\mathcal{KD}_{\alpha,1} = \mathcal{X}_\alpha$, the results for the Pl_α index follow directly from Theorem 2.15.

In conclusion, the $\mathcal{KD}_{\alpha,\beta}$ index, with its flexibility in α and β, generalizes many degree-based indices, some are illustrated in Table 1. This highlights its potential for exploring various graph parameters in future studies.

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