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Retraction

Retracted: On Vertex Degree-Based Topological Indices for Fixed Branching Vertices of Trees

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This article has been retracted by Hindawi, as publisher, following an investigation undertaken by the publisher [1]. This investigation has uncovered evidence of systematic manipulation of the publication and peer-review process. We cannot, therefore, vouch for the reliability or integrity of this article.

Please note that this notice is intended solely to alert readers that the peer-review process of this article has been compromised.

Wiley and Hindawi regret that the usual quality checks did not identify these issues before publication and have since put additional measures in place to safeguard research integrity.

We wish to credit our Research Integrity and Research Publishing teams and anonymous and named external researchers and research integrity experts for contributing to this investigation.

The corresponding author, as the representative of all authors, has been given the opportunity to register their agreement or disagreement to this retraction. We have kept a record of any response received.

References

[1] M. Hanif, A. A. Bhatti, M. Javaid, and M. N. Alam, “On Vertex Degree-Based Topological Indices for Fixed Branching Vertices of Trees,” *Journal of Chemistry*, vol. 2022, Article ID 3642849, 8 pages, 2022.

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Research Article

On Vertex Degree-Based Topological Indices for Fixed Branching Vertices of Trees

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The Gourava indices and hyper-Gourava indices are graph invariants, related to the degree of vertices of a graph G. Let $\mathbb{T}_{n,b}$ denote the collection of all chemical trees with n vertices where b denotes the number of branching vertices, $1 \le b < (n-2)/2$. In the current paper, maximum value for the abovementioned topological indices for different classes ${}^1\mathbb{T}_{n,b}$ and ${}^2\mathbb{T}_{n,b}$ of $\mathbb{T}_{n,b}$ is determined and the corresponding extremal trees are characterized.

1. Introduction

In this paper, we only consider simple, finite, and connected graphs. Let G be a simple graph of order n with vertex set $V(G) = \{v_i, i = 1,2,3,. \cdots, n\}$ and edge set $E(G) = \{e_j, j = 1,2,3,. \cdots, m\}$. Let $N_u(G)$ be the neighborhood set of the vertex u in graph G. The number of adjacent vertices to a vertex u is said to be its degree, and it is denoted by d_u. The adjacency of two vertices u and v is denoted by $u \sim v$. In a graph G, the vertices of degree one and the degree greater or equal to three are known as pendent (leaf) and branching vertices, respectively. A pendent vertex u is said to be a starlike pendent vertex if it is connected to a branching vertex v. Let P_n and S_n be the path and star graph of order n, respectively. A path which contains single pendent vertex is known as pendent path whereas if both ending vertices are branching in a path, then it is known as *internal path* [1]. A vertex degree-based topological index is a function $\widehat{TI} : \mathbb{T}_{n,b} \longrightarrow \mathbb{R}$ induced by numbers $\{\varphi_{(i,j)}\}_{(i,j)\in \Upsilon}$, defined for every tree $T \in \mathbb{T}_{n,b}$ as [2]

$$\widehat{TI}(T) = \sum_{(i,j)\in\Upsilon} \varrho_{i,j}(T)\,\varphi_{(i,j)}, \tag{1}$$

where $\Upsilon = \{(i,j) \in \mathbb{N}\times\mathbb{N} : 1 \le i \le j \le 4\}$, and $\varrho_{i,j}$ be the number of edges of vertices having degrees i and j.

Topological indices are studied intensively in recent years and among the oldest and the most studied being the first and second Zagreb indices $M_1(G)$ and $M_2(G)$, respectively. In 1972, Gutman and Trinajstić defined the first and second Zagreb indices as [3, 4]

$$\begin{aligned} M_1(G) &= \sum_{v\in V(G)} d_v^2(G), \\ M_2(G) &= \sum_{u\sim v} d_u(G) d_v(G). \end{aligned} \tag{2}$$

The first Zagreb index is also defined as [5]

$$M_1(G) = \sum_{u\sim v} [d_u(G) + d_v(G)]. \quad (3)$$

For the minimum first Zagreb index, trees have been characterized with respect to a fixed number of pendent vertices by Gutman and Goubko [6, 7]. Lin [8] maximized and minimized the first Zagreb index of the trees with respect to a fixed number of segments. After that, Borovićanin et al. [9–11] characterized certain classes of trees with maximum and minimum Zagreb indices with a fixed number of segments or branching vertices. In 2013, the upper bounds on the multiplicative Zagreb indices of Cartesian product, the join, composition, corona product, and disjunction of graphs have been derived by Das et al. [12]. In 2016, Das et al. [13] established some upper and lower bounds on the first Zagreb index of graphs and trees in terms of irregularity index, a number of vertices, and maximum degree and have characterized the extremal graphs. In 2016, the relations among Zagreb polynomials on three graph operators have been discussed by Bindusree et al. [14]. After that in 2019, Aykaç et al. [15] established first Zagreb index, second Zagreb index, first multiplicative Zagreb index, second multiplicative Zagreb index, first Zagreb coindices index, second Zagreb coindices index, first multiplicative Zagreb coindices index, and second multiplicative Zagreb coindices index of $\Gamma(\mathbb{Z}_{p^2} \times \mathbb{Z}_{q^2})$. Recently, Noreen et al. [1] characterized the n-vertex trees for maximum Zagreb indices with a fixed number of segments or branching vertices. For more details, see [1, 3, 4, 6, 7, 9–11, 16–26].

In 2011, Azari and Iranmanesh [27] defined the generalized Zagreb index of graphs as

$$M_{\alpha,\beta}(G) = \sum_{u\sim v} \left[(d_u(G))^{\alpha} (d_v(G))^{\beta} + (d_u(G))^{\beta} (d_v(G))^{\alpha} \right], \forall \alpha, \beta \in \mathbb{N}. \quad (4)$$

Motivated by the first and second Zagreb indices and their various applications in the different disciplines, Kulli [28] defined the first Gourava index of a graph G as

$$GO_1(G) = \sum_{u\sim v} [(d_u(G) + d_v(G)) + d_u(G) d_v(G)]. \quad (5)$$

Then, by motivation of the generalized Zagreb index and the first Gourava index, Kulli defined the second Gourava index as [28]

$$GO_2(G) = \sum_{u\sim v} [(d_u(G) + d_v(G))(d_u(G) d_v(G))], \quad (6)$$

which is also written in the form of generalized Zagreb index as

$$GO_2(G) = \sum_{u\sim v} \left[(d_u(G))^2 d_v(G) + d_u(G)(d_v(G))^2 \right], \quad (7)$$

and computed the first and second Gourava indices, the multiplicative first and second Gourava indices, and general multiplicative first and second Gourava indices of armchair polyhex and zigzag-edge polyhex nanotubes. After that, Kulli defined first and second hyper-Gourava indices as [29]

$$HGO_1(G) = \sum_{u\sim v} [(d_u(G) + d_v(G)) + d_u(G) d_v(G)]^2, \quad (8)$$

$$HGO_2(G) = \sum_{u\sim v} [(d_u(G) + d_v(G))(d_u(G) d_v(G))]^2, \quad (9)$$

and computed the first and second hyper-Gourava indices of $HC_5C_7[p, q]$, $SC_5C_7[p, q]$ nanotubes. In 2021, Aftab et al. [30] computed the different topological indices such as the first and second Gourava indices and the first and second hyper-Gourava indices of subdivided hexagonal network, subdivided polythiophene network, subdivided honeycomb network, and subdivided backbone DNA network.

The abovementioned indices have good correlation with physical properties of chemical compounds like entropy (S), acentric factor (AcentFac), and standard enthalpy of vaporization (DHVAP) of octane isomers. GO_1 index correlates highly with entropy, and the correlation coefficient is $|r| = 0.9644924$. Also, GO_1 index has good correlation ($|r| > 0.9$) with acentric factor and ($|r| > 0.8$) with the standard enthalpy of vaporization. GO_2 index correlates highly with acentric factor, and the correlation coefficient is $|r| = 0.9644924$. Also, GO_2 index has good correlation ($|r| > 0.9$) with entropy and ($|r| > 0.75$) with the standard enthalpy of vaporization. HGO_1 index correlates highly with acentric factor, and the correlation coefficient is $|r| = 0.9554303$. Also, HGO_1 index has good correlation ($|r| > 0.9$) with entropy and ($|r| > 0.75$) with the standard enthalpy of vaporization. HGO_2 index has good correlation ($|r| > 0.85$) with entropy, ($|r| > 0.75$) with acentric factor, and ($|r| > 0.6$) with the standard enthalpy of vaporization. For more detail about the fitted models for the abovementioned indices, see [31].

It is noted that for any $T \in \mathbb{T}_{n,(n-2)/2}$, it contains only vertices of degree one and three. So we let ${}^1\mathbb{T}_{n,b}$, $1 \le b < (n-2)/3$ and ${}^2\mathbb{T}_{n,b}$, $(n-2)/3 \le b < (n-2)/2$ be two subclasses of $\mathbb{T}_{n,b}$ with degree sequences $(\underbrace{4, 4, \cdots, 4}_{b}, \underbrace{2, 2, \cdots, 2}_{n-3b-2}, \underbrace{1, 1, \cdots, 1}_{2b+2})$ and $(\underbrace{4, 4, \cdots, 4}_{n-2b-2}, \underbrace{3, 3, \cdots, 3}_{3b-n+2}, \underbrace{1, 1, \cdots, 1}_{n-b})$, respectively. Let $V_i(G)$ be the number of vertices of degree $i, 1 \le i \le 4$ in G. For chemical trees, the following relations are well known, where $1 \le j \le 4$ and $\Delta = 4$.

$$2\varrho_{j,j} + \sum_{\substack{i=1 \\ i \ne j}}^{\Delta} \varrho_{j,i} = jV_j, \quad (10)$$

$$\sum_{1 \le i \le j \le \Delta} \varrho_{i,j} = n - 1. \quad (11)$$

From (10), we have following system of equations:

$$2\varrho_{1,1} + \varrho_{1,2} + \varrho_{1,3} + \varrho_{1,4} = V_1, \tag{12}$$

$$\varrho_{2,1} + 2\varrho_{2,2} + \varrho_{2,3} + \varrho_{2,4} = 2V_2, \tag{13}$$

$$\varrho_{3,1} + \varrho_{3,2} + 2\varrho_{3,3} + \varrho_{3,4} = 3V_3, \tag{14}$$

$$\varrho_{4,1} + \varrho_{4,2} + \varrho_{4,3} + 2\varrho_{4,4} = 4V_4. \tag{15}$$

2. Main Result

Let ${}^1T_{\max} \in {}^1\mathbb{T}_{n,b}$ and ${}^2T_{\max} \in {}^2\mathbb{T}_{n,b}$ be the maximal trees, which maximize the abovementioned indices. For this, we determine the structures of ${}^1T_{\max}$ and ${}^2T_{\max}$ from the following lemmas.

Lemma 1. *Let ${}^2T_{\max} \in \mathbb{T}_{n,b}$ with $1 \le b < (n-2)/2$ be a maximal tree. Then, it contains internal path of length one only.*

Proof. Suppose, to the contrary, that ${}^2T_{\max}$ has an internal path of length greater than or equal to two. Let be an internal path of length greater than or equal to two in ${}^2T_{\max}$ where u_1 and u_k be the branching vertices and $\forall d_{u_j} = 2, 1 < j < k$. Let a leaf w be adjacent to some vertex u_i other than $u_j, 1 < j < k$. Let $T^* = {}^2T_{\max} - \{u_i w, u_1 u_2, u_{k-1} u_k\} + \{u_1 u_k, u_2 w, u_{k-1} u_i\}$; then, $T^* \in \mathbb{T}_{n,b}$ and

$$\begin{aligned}
&GO_1({}^2T_{\max}) - GO_1(T^*) = 4d_{u_k} - d_{u_1} - d_{u_1} d_{u_k} - 8 < 0, \left(\text{since } 3 \le d_{u_k} < d_{u_1}\right),\\
&GO_2({}^2T_{\max}) - GO_2(T^*) = -d_{u_1}^2\left(d_{u_k} + 1\right) - d_{u_1}\left(d_{u_k}^2 + 7\right)\\
&\qquad + 4d_{u_k}^2 + 6d_{u_k} - 34 < 0, \left(\text{since } 3 \le d_{u_k} < d_{u_1}\right),\\
&HGO_1({}^2T_{\max}) - HGO_1(T^*) = -d_{u_1}^2\left(d_{u_k}^2 + 11\right) - d_{u_1}\left(4d_{u_k}^2 - 2d_{u_k} + 32\right)\\
&\qquad + 2\left(9d_{u_k}^2 + 8d_{u_k} - 64\right) < 0, \left(\text{since } 3 \le d_{u_k} < d_{u_1}\right),\\
&HGO_2({}^2T_{\max}) - HGO_2(T^*) = -d_{u_1}^4\left(d_{u_k}^2 - 2d_{u_k} + 9\right) - 2d_{u_1}^3\left(d_{u_k}^3 - d_{u_k}^2 - d_{u_k} + 39\right)\\
&\quad - d_{u_1}^2\left(d_{u_k}^4 + 2d_{u_k}^3 - 6d_{u_k}^2 + 2d_{u_k} + 269\right) - 2d_{u_1}\left(d_{u_k}^4 - d_{u_k}^3 - d_{u_k}^2 + d_{u_k} + 170\right)\\
&\quad + 10d_{u_k}^4 + 28d_{u_k}^3 + 30d_{u_k}^2 - 924, < 0, \left(\text{since } \quad 3 \le d_{u_k} < d_{u_1}\right),
\end{aligned} \tag{16}$$

a contradiction to ${}^2T_{\max}$, due to the fact $d_{u_1} \ge 4$ and $d_{u_k} \ge 3$. Hence, ${}^2T_{\max}$ contains internal path of length one only. □

Lemma 2. *Let ${}^2T_{\max} \in \mathbb{T}_{n,b}$ with $1 \le b < (n-2)/2$ be a maximal tree. If ${}^2T_{\max}$ contains $\varrho_{1,i} \ne 0, 2 < i \le 4$, then it contains pendent path of length at most two.*

Proof. Suppose, to the contrary, that ${}^2T_{\max}$ has an pendent path of length greater than or equal to three. Let be a pendent path of length greater than or equal to three and a leaf w is connected to u in ${}^2T_{\max}$ where u is a branching vertex. Then, we have another tree $T^* = {}^2T_{\max} - \{uw, u_1u_2, u_2u_3\} + \{u_2w, u_2u, u_1u_3\}$ such that $T^* \in \mathbb{T}_{n,b}$ and

$$\begin{aligned}
&GO_1({}^2T_{\max}) - GO_1(T^*) = 2 - d_u < 0, (\text{since } d_u \ge 3),\\
&GO_2({}^2T_{\max}) - GO_2(T^*) = 10 - 3d_u - d_u^2 < 0, (\text{since } d_u \ge 3),\\
&HGO_1({}^2T_{\max}) - HGO_1(T^*) = 36 - 8d_u - 5d_u^2 < 0, (\text{since } d_u \ge 3),\\
&HGO_2({}^2T_{\max}) - HGO_2(T^*) = 220 - 15d_u^2 - 14d_u^3 - 3d_u^4 < 0, (\text{since } d_u \ge 3),
\end{aligned} \tag{17}$$

a contradiction to ${}^2T_{\max}$. Hence, ${}^2T_{\max}$ contains a pendent path of length at most two. □

Lemma 3. *Let ${}^1T_{\max} \in \mathbb{T}_{n,b}$ (respectively ${}^2T_{\max} \in \mathbb{T}_{n,b}$) with $1 \le b < (n-2)/2$ be a maximal tree. If it contains $\varrho_{2,i}, i \in \{1, 2, 4\}$, then it does not contain $\varrho_{3,j}, j \in \{1, 3, 4\}$ and vice versa.*

Proof. Suppose, to the contrary, that ${}^1T_{\max}$ (respectively ${}^2T_{\max}$) has $\varrho_{2,i}, \varrho_{3,i}, i \in \{1,2,3,4\}$. This means it contains vertices of degrees two and three simultaneously. Let a branching vertex u of degree three be adjacent to its neighbor vertices u_1, u_2 and $u_3(= v)$ with $d_{u_1} \ge 1$ and $d_{u_2} \ge 1$. Let v be a vertex of degree two which is adjacent to its neighbor vertices u and x. We obtained another tree $T^* = {}^2T_{\max} - \{uu_1, uu_2\} + \{vu_1, vu_1\}$ such that $T^* \in \mathbb{T}_{n,b}$ and

$$\begin{aligned}
&GO_1({}^1T_{\max}) - GO_1(T^*) = -6 - \left(d_{u_1} + d_{u_2}\right) < 0,\\
&GO_2({}^1T_{\max}) - GO_2(T^*) = -22 - 7\left(d_{u_1} + d_{u_2}\right) - \left(d_{u_1}^2 + d_{u_1}^2\right) < 0,\\
&HGO_1({}^1T_{\max}) - HGO_1(T^*) = -106 - 16\left(d_{u_1} + d_{u_2}\right) - 9\left(d_{u_1}^2 + d_{u_2}^2\right) < 0,\\
&HGO_2({}^1T_{\max}) - HGO_2(T^*) = -1548 - 175\left(d_{u_1}^2 + d_{u_2}^2\right) - 74\left(d_{u_1}^3 + d_{u_2}^3\right) - 7\left(d_{u_1}^4 + d_{u_2}^4\right), < 0,
\end{aligned} \tag{18}$$

a contradiction to the choice of ${}^1T_{\max}$ (respectively ${}^2T_{\max}$). Hence, ${}^1T_{\max}$ (respectively ${}^2T_{\max}$) has no vertices of degrees two and three simultaneously. □

Lemma 4. *For any tree $T_{\max} \in \mathbb{T}_{n,b}$ with $1 \le b < (n-2)/2$, the following result holds.*

$$DS(T_{\max}) = \begin{cases} \left(\underbrace{4, 4, \cdots, 4}_{b}, \underbrace{2, 2, \cdots, 2}_{n-3b-2}, \underbrace{1, 1, \cdots, 1}_{2b+2}\right) & \text{if } T_{\max} \in {}^1\mathbb{T}_{n,b},\\ \left(\underbrace{4, 4, \cdots, 4}_{n-2b-2}, \underbrace{3, 3, \cdots, 3}_{3b-n+2}, \underbrace{1, 1, \cdots, 1}_{n-b}\right) & \text{if } T_{\max} \in {}^2\mathbb{T}_{n,b}. \end{cases} \tag{19}$$

Proof. Let $T_{\max}$ be a maximal tree in $\mathbb{T}_{n,b}$. To find the number of vertices of different degrees of the abovementioned degree sequences, we have two cases:

Case: 1

If $V_3 = 0$, then $V_4 = b$ are total branching vertices in $T_{\max}$. Since $V_2 > 0$ and with the help of some already recorded results $n = \sum_{i=1}^{\Delta} V_i$ and $2(n-1) = \sum_{i=1}^{\Delta} iV_i$, we get $V_1 = 2b + 2$ and $V_2 = n - V_4 - V_1 = n - 3b - 2$.

Case: 2

If $V_3 > 0$, then $V_3 + V_4 = b$ are the branching vertices in $T_{\max}$. Since $V_2 = 0$, it is noted that there are $n - b$ pendent vertices in $T_{\max}$. Again using the above results $n = \sum_{i=1}^{\Delta} V_i$ and $2(n-1) = \sum_{i=1}^{\Delta} iV_i$, we get $V_3 = 3b - n + 2$ and $V_4 = n - 2b - 2$. □

Lemma 5. *Let ${}^1T_{\max} \in \mathbb{T}_{n,b}$ (respectively ${}^2T_{\max} \in \mathbb{T}_{n,b}$) with $1 \le b < (n-2)/2$ be a maximal tree. It contains $\varrho_{2,i}$, $i \in \{1, 2, 4\}$ iff $1 \le b < (n-2)/3$.*

Proof. Let ${}^1T_{\max}$ be a maximal tree with $1 \le b < (n-2)/3$. Then, by Lemmas 3 and 4, ${}^1T_{\max}$ has $\varrho_{2,i}$, $i \in \{1,2,4\}$. So, it has at least one vertex of degree two. Also, by Lemma 3, there is no vertex of degree three in ${}^1T_{\max}$. So $V_2 = n - 3b - 2 \ge 1$ which gives $3b \le n - 3 < n - 2$. Hence, $b < (n-2)/3$. Conversely, let $1 \le b < (n-2)/3$; this implies $n \ge 3b + 3 > 3b + 2$ and $1 \le b$. By using induction technique on b, we will show that there exists a vertex of degree two at least. For $b = 1$, we have $n > 5$ and it will be a starlike tree with a degree of branching vertex is four. Now assume that result is also true for $b = k$, and we have $n \ge 3k + 3$ with k branching vertices where $k \ge 1$. Now we have to prove that it will be true for $b = k + 1$. For this, let ${}^1T_{\max}$ be a tree of order $n \ge 3(k+1) + 3$ with $k + 1$ number of branching vertices with a maximum degree of any branching vertex at most four. Let $P : u_0u_1u_2 \cdots u_{l-1}u_l$ be a longest path in ${}^1T_{\max}$ with u_1 be a branching vertex of degree at most four. We note that all neighbors of u_1 be pendent vertices except u_2. We obtained another tree T^* after deleting all those pendent paths related to u_1. It means T^* has $(k+1) - 1 = k$ branching vertices. So T^* has order $n \ge 3k + 3$. Hence, T^* has at least one vertex of degree two. Thus, ${}^1T_{\max}$ also has a degree two vertex at least. By induction, this completes the proof. □

Lemma 6. *Let ${}^2T_{\max} \in \mathbb{T}_{n,b}$ with $1 \le b < (n-2)/2$ be a maximal tree. If it contains $\varrho_{1,4} \ne 0$, then it has no $\varrho_{3,3}$ in ${}^2T_{\max}$.*

Proof. Suppose, to the contrary, that ${}^2T_{\max}$ has both $\varrho_{3,3}$ and $\varrho_{1,4}$. This means there are two vertices, say x, y, of degree three, and also, a leaf v is connected to a vertex w of degree four in ${}^2T_{\max}$. Assume that there is a unique path $v - x$ that contains vertex y. Let x_i, $1 \le i \le 2$ be the neighbors of vertex x different from y. If we obtained another tree $T^* = {}^2T_{\max} - \{xx_1, xx_2\} + \{vx_1, vx_2\}$, then ${}^2T_{\max} \in \mathbb{T}_{n,b}$ and we have $GO_1({}^2T_{\max}) - GO_1(T^*) = -2 < 0$, $GO_2({}^2T_{\max}) - GO_2(T^*) = -22 < 0$, $HGO_1({}^2T_{\max}) - HGO_1(T^*) = -104 < 0$, and $HGO_2({}^2T_{\max}) - HGO_2(T^*) = -3884 < 0$, which is a contradiction to the choice of ${}^2T_{\max}$. Hence, if ${}^2T_{\max}$ contains $\varrho_{1,4} \ne 0$, then, it has no $\varrho_{3,3}$ in ${}^2T_{\max}$. □

Lemma 7. *Let ${}^2T_{\max} \in \mathbb{T}_{n,b}$ with $1 \le b < (n-2)/2$ be a maximal tree. Then, every vertex having degree three in ${}^2T_{\max}$ is connected to one vertex at most, having degree four.*

Proof. Suppose, to the contrary, that a vertex w of degree three is adjacent to its neighbors u and v of degree four each. By Lemma 3, there is no $\varrho_{2,i}$ in ${}^2T_{\max}$ which means it has no vertex of degree two. Let a leaf x be connected to branching vertex v or u other than w. Then, a tree T^* is obtained by deleting edges uw, vw, xv and adding edges uv, wx, vw; then, $T^* \in \mathbb{T}_{n,b}$, and we get $GO_1({}^2T_{\max}) - GO_1(T^*) = -3 < 0$, $GO_2({}^2T_{\max}) - GO_2(T^*) = -36 < 0$, $HGO_1({}^2T_{\max}) - HGO_1(T^*) = -183 < 0$, and $HGO_2({}^2T_{\max}) - HGO_2(T^*) = -9072 < 0$, a contradiction to the choice of ${}^2T_{\max}$. Hence, we have the required result. □

Lemma 8. *Let ${}^2T_{\max} \in \mathbb{T}_{n,b}$ with $1 \le b < (n-2)/2$ be a maximal tree. Then, it must contain vertex/vertices of degree four, and the induced graph from the vertex/vertices of degree four is a tree.*

Proof. If $1 \le b < n - 2/3$, then by Lemma 5, we have at least one branching vertex, i.e., $1 \le b$, and by Lemma 3, ${}^1T_{\max}$ (respectively ${}^2T_{\max}$) has no vertices of degrees two and three at a time. Also by Lemma 4, ${}^1T_{\max}$ has no vertex of degree three so that the only branching vertices are the vertices of degree four, i.e., $V_4 \ge 1$. By Lemma 1, the induced graph from the vertex/vertices of degree four is a tree. Now if $n - 2/3 \le b < n - 2/2$, then by Lemma 4, ${}^2T_{\max}$ has no vertex of degree two and by Lemma 5, we have $V_4 = n - 2b - 2$. It follows $V_4 \ge 1$. Hence, by Lemma 1, we have the required result. □

Theorem 9. *Let $T_{\max} \in {}^1\mathbb{T}_{n,b}$, where $1 \le b < (n-2)/3$; then, for $(\underbrace{4, 4, \cdots, 4}_{b}, \underbrace{2, 2, \cdots, 2}_{n-3b-2}, \underbrace{1, 1, \cdots, 1}_{2b+2})$,*

$$
\begin{aligned}
GO_1(T_{\max}) &\le \begin{cases} 8n + 22b - 18 & 1 \le b < \dfrac{n-4}{5}, \\ 10n + 12b - 26 & \dfrac{n-4}{5} \le b < \dfrac{n-2}{3}, \end{cases} \\
GO_2(T_{\max}) &\le \begin{cases} 16n + 156b - 84 & 1 \le b < \dfrac{n-4}{5}, \\ 34n + 66b - 156 & \dfrac{n-4}{5} \le b < \dfrac{n-2}{3}, \end{cases} \\
HGO_1(T_{\max}) &\le \begin{cases} 64n + 698b - 390 & 1 \le b < \dfrac{n-4}{5}, \\ 140n + 318b - 694 & \dfrac{n-4}{5} \le b < \dfrac{n-2}{3}, \end{cases} \\
HGO_2(T_{\max}) &\le \begin{cases} 256n + 19784b - 12728 & 1 \le b < \dfrac{n-4}{5}, \\ 1940n + 11364b - 19464 & \dfrac{n-4}{5} \le b < \dfrac{n-2}{3}. \end{cases}
\end{aligned}
\tag{20}
$$

The equality holds iff $T_{\max}$ has degree sequence ($\underbrace{4,4,\cdots,4}_{b},\underbrace{2,2,\cdots,2}_{n-3b-2},\underbrace{1,1,\cdots,1}_{2b+2}$).

Proof. By Lemma 8, we have $\varrho_{4,4}=V_4-1=b-1$. Now if $1\leq b<(n-2)/3$, then we have two cases:

Case 1. If $1\leq b<(n-4)/5$, then $\varrho_{1,4}=0$. From (12)–(15), we get $\varrho_{1,2}=\varrho_{2,4}=2b+2, \varrho_{2,2}=n-5b-4$. Then, (9) becomes

$$\begin{aligned}\widehat{TI}(T_{\max})&=\varrho_{1,2}\varphi(1,2)+\varrho_{1,4}\varphi(1,4)+\varrho_{2,2}\varphi(2,2)+\varrho_{2,4}\varphi(2,4)+\varrho_{4,4}\varphi(4,4),\\&=(2b+2)\varphi(1,2)+(n-5b-4)\varphi(2,2)+(2b+2)\varphi(2,4)+(b-1)\varphi(4,4),\\&=(2b+2)(\varphi(1,2)+\varphi(2,4))+(n-5b-4)\varphi(2,2)+(b-1)\varphi(4,4).\end{aligned}\tag{21}$$

It follows

$$\begin{aligned}GO_1(T_{\max})&=24(b-1)+38(b+1)+8(n-5b-4),=8n+22b-18,\\GO_2(T_{\max})&=128(b-1)+108(b+1)+16(n-5b-4),=16n+156b-84,\\HGO_1(T_{\max})&=576(b-1)+442(b+1)+64(n-5b-4),=64n+698b-390,\\HGO_2(T_{\max})&=16384(b-1)+4680(b+1)+256(n-5b-4),\\&=256n+19784b-12728.\end{aligned}\tag{22}$$

Case 2. For $(n-4)/5\leq b<(n-2)/3$, if $\varrho_{1,4}\neq 0$, then by Lemmas 1 and 2, we have $\varrho_{2,2}=0$. From (12)–(15), we get $\varrho_{1,2}=\varrho_{2,4}=n-3b-2, \varrho_{2,2}=0, \varrho_{1,4}=5b-n+4$. Then, (9) becomes

$$\begin{aligned}\widehat{TI}(T_{\max})&=\varrho_{1,2}\varphi(1,2)+\varrho_{1,4}\varphi(1,4)+\varrho_{2,2}\varphi(2,2)+\varrho_{2,4}\varphi(2,4)+\varrho_{4,4}\varphi(4,4),\\&=(n-3b-2)\varphi(1,2)+(5b-n+4)\varphi(1,4)+(n-3b-2)\varphi(2,4)\\&\quad+(b-1)\varphi(4,4),=(n-3b-2)(\varphi(1,2)+\varphi(2,4))\\&\quad+(5b-n+4)\varphi(1,4)+(b-1)\varphi(4,4).\end{aligned}\tag{23}$$

It follows

$$\begin{aligned}GO_1(T_{\max})&=24(b-1)+9(5b-n+4)+19(n-3b-2),=10n+12b-26,\\GO_2(T_{\max})&=128(b-1)+20(5b-n+4)+54(n-3b-2),=34n+66b-156,\\HGO_1(T_{\max})&=576(b-1)+81(5b-n+4)+221(n-3b-2),=140n+318b-694,\\HGO_2(T_{\max})&=16384(b-1)+400(5b-n+4)+2340(n-3b-2),\\&=1940n+11364b-19464,\end{aligned}\tag{24}$$

which completes the proof. □

In Figure 1, for $n=20$, three trees $T_{20,1}$, $T_{20,2}$, and $T_{20,3}$, having 1, 2, and 3 branching vertices, respectively, are in ${}^{1}\mathbb{T}_{20,b}$ where $1\leq b<(n-4)/5$ and satisfies Theorem 9, Case 1. And next two trees $T_{20,4}$ and $T_{20,5}$, having 4 and 5 branching vertices, respectively, are in ${}^{1}\mathbb{T}_{20,b}$ where $(n-4)/5\leq b<(n-2)/3$ and satisfies Theorem 9, Case 2.

Theorem 10. *Let $T_{\max}\in{}^{2}\mathbb{T}_{n,b}$, where $(n-2)/3\leq b\leq(n-2)/2$; then, for ($\underbrace{4,4,\cdots,4}_{n-2b-2},\underbrace{3,3,\cdots,3}_{3b-n+2},\underbrace{1,1,\cdots,1}_{n-b}$),*

$$GO_1(T_{\max})\leq\begin{cases}18n-12b-42 & \frac{n-2}{3}\leq b<\frac{3n-4}{7},\\24n-26b-50 & \frac{3n-4}{7}\leq b<\frac{n-2}{2},\end{cases}$$

$$GO_2(T_{\max})\leq\begin{cases}80n-72b-248 & \frac{n-2}{3}\leq b<\frac{3n-4}{7},\\146n-226b-336 & \frac{3n-4}{7}\leq b<\frac{n-2}{2},\end{cases}$$

$$HGO_1(T_{\max})\leq\begin{cases}360n-342b-1134 & \frac{n-2}{3}\leq b<\frac{3n-4}{7},\\672n-1070b-1550 & \frac{3n-4}{7}\leq b<\frac{n-2}{2},\end{cases}$$

$$HGO_2(T_{\max})\leq\begin{cases}10240n-13536b-36064 & \frac{n-2}{3}\leq b<\frac{3n-4}{7},\\21892n-40724b-51600 & \frac{3n-4}{7}\leq b<\frac{n-2}{2}.\end{cases}\tag{25}$$

The equality holds iff $T_{\max}$ has degree sequence ($\underbrace{4,4,\cdots,4}_{n-2b-2},\underbrace{3,3,\cdots,3}_{3b-n+2},\underbrace{1,1,\cdots,1}_{n-b}$).

Proof. Again by Lemma 8, we have $\varrho_{4,4}=V_4-1=b-1$. If $(n-2)/3\leq b<(n-2)/2$, then we have two cases:

Case 1. For $(n-2)/3\leq b<(3n-4)/7$, if $\varrho_{1,4}\neq 0$, then by Lemma 6, $\varrho_{3,3}=0$. From (12)–(15), we get $\varrho_{1,3}=6b-2n+4$, $\varrho_{1,4}=3n-7b-4$, $\varrho_{3,4}=3b-n+2$. Then, (9) becomes

$$\begin{aligned}\widehat{TI}(T_{\max})&=\varrho_{1,3}\varphi(1,3)+\varrho_{1,4}\varphi(1,4)+\varrho_{3,3}\varphi(3,3)+\varrho_{3,4}\varphi(3,4)\\&\quad+\varrho_{4,4}\varphi(4,4),=(6b-2n+4)\varphi(1,3)+(3n-7b-4)\varphi(1,4)\\&\quad+(3b-n+2)\varphi(3,4)+(n-2b-3)\varphi(4,4).\end{aligned}\tag{26}$$

It follows

$$\begin{aligned}GO_1(T_{\max})&=33(3b-n+2)+24(n-2b-3)+9(3n-7b-4),\\&=18n-12b-42,\\GO_2(T_{\max})&=108(3b-n+2)+128(n-2b-3)+20(3n-7b-4),\\&=80n-72b-248,\end{aligned}$$

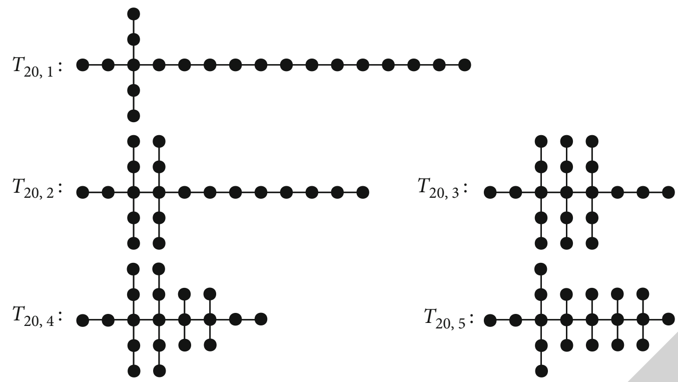

Figure 1: Five trees in the class of ${}^1\mathbb{T}_{20,b}$ where $1 \le b < (n-2)/3$.

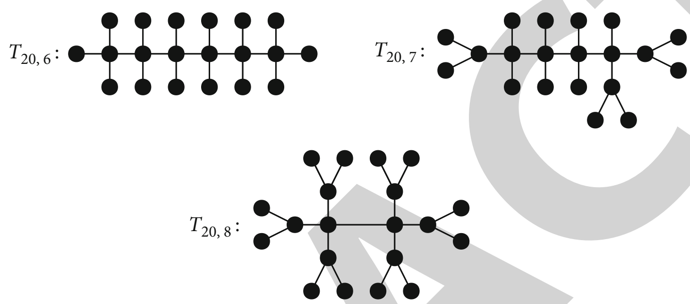

Figure 2: Three trees in the class of ${}^2\mathbb{T}_{20,b}$ where $(n-2)/3 \le b < (n-2)/2$.

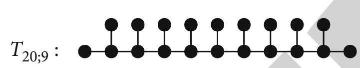

Figure 3: One tree in the class of $\mathbb{T}_{20,b}$ where $b = (n-2)/2$.

$$HGO_1(T_{\max}) = 459(3b-n+2) + 576(n-2b-3) + 81(3n-7b-4), = 360n - 342b - 1134,$$

$$HGO_2(T_{\max}) = 7344(3b-n+2) + 16384(n-2b-3) + 400(3n-7b-4), = 10240n - 13536b - 36064. \quad (27)$$

Case 2. For $(3n-4)/7 \le b < (n-2)/2$, if $\varrho_{1,4} = 0$, then by Lemma 6, $\varrho_{3,3} \neq 0$. From (12)–(15), we get $\varrho_{1,3} = n-b$, $\varrho_{3,3} = 7b-3n+4$, $\varrho_{3,4} = 2n-4b-2$. Then, (9) becomes

$$\widehat{TI}(T_{\max}) = \varrho_{1,3}\varphi(1,3) + \varrho_{1,4}\varphi(1,4) + \varrho_{3,3}\varphi(3,3) + \varrho_{3,4}\varphi(3,4) + \varrho_{4,4}\varphi(4,4), = (n-b)\varphi(1,3) + (7b-3n+4)\varphi(3,3) + (2n-4b-2)\varphi(3,4) + (n-2b-3)\varphi(4,4). \quad (28)$$

It follows

$$GO_1(T_{\max}) = 15(7b-3n+4) - 38(2b-n+1) + 24(n-2b-3) + 7(n-b), = 24n - 26b - 50,$$

$$GO_2(T_{\max}) = 54(7b-3n+4) - 168(2b-n+1) + 128(n-2b-3) + 12(n-b), = 146n - 226b - 336,$$

$$HGO_1(T_{\max}) = 225(7b-3n+4) - 722(2b-n+1) + 576(n-2b-3) + 49(n-b), = 672n - 1070b - 1550,$$

$$HGO_2(T_{\max}) = 2916(7b-3n+4) - 14112(2b-n+1) + 16384(n-2b-3) + 144(n-b), = 21892n - 40724b - 51600, \quad (29)$$

which completes the proof. □

In Figure 2, for $n = 20$, two trees $T_{20,6}$ and $T_{20,7}$, having 6 and 7 branching vertices, respectively, are in ${}^2\mathbb{T}_{20,b}$ where $(n-2)/3 \le b < (3n-4)/7$ and satisfies Theorem 10, Case 1. And next one tree $T_{20,8}$, having 8 branching vertices, is in ${}^2\mathbb{T}_{20,b}$ where $(3n-4)/7 \le b < (n-2)/2$ and satisfies Theorem 10, Case 2.

In Figure 3, for $n = 20$, one tree $T_{20,9}$ having 9 branching vertices, is in $\mathbb{T}_{20,b}$ where $b = (n-2)/2$ and this tree contains only vertices of degree one and three.

3. Conclusions

Topological indices are the main tool for investigating the properties of different molecular descriptors by many researchers in the last decade. We have determined sharp upper bonds on the Gourava indices and hyper-Gourava indices with a fixed number of branching vertices for the classes of n-vertex chemical trees ${}^{1}\mathbb{T}_{n,b}$ and ${}^{2}\mathbb{T}_{n,b}$ of $\mathbb{T}_{n,b}$. The above-computed graph invariants are used as molecular descriptors in the construction of the theoretical models such as quantitative structure-activity relationships (QSARs) which relate the quantitative measure of a chemical structure to a biological property or a physical property and quantitative structure-property relationships (QSPRs) which relate mathematically physical/chemical properties to the structure of a molecule. The above results can be correlated with the physical properties like entropy, acentric factor, and standard enthalpy of vaporization, of hydrocarbons. We have given nine examples of the chemical graphs that can be verified by using the results of Theorems 9 and 10. At this stage, we left the lower bonds on the abovementioned indices for the collection of all chemical trees with n vertices and b branching vertices for the abovementioned classes as an open problem.

Data Availability

The whole data are included within this article. However, the reader may contact the corresponding author for more details on the data.

Conflicts of Interest

The authors declare no conflicts of interest.

References

[1] S. Noureen, A. Ali, and A. A. Bhatti, "On the extremal Zagreb indices of n- vertex chemical trees with fixed number of segments or branching vertices," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 84, pp. 513–534, 2020.

[2] R. Cruz, J. Monsalve, and J. Rada, "On chemical trees that maximize atom-bond connectivity index, its exponential version, and minimize geometric-arithmetic index," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 84, pp. 691–718, 2020.

[3] I. Gutman and N. Trinajstić, "Graph theory and molecular orbitals. Total π- electron energy of alternant hydrocarbons," *Chemical Physics Letters*, vol. 17, pp. 535–538, 1972.

[4] I. Gutman, B. Ruščić, N. Trinajstić, and C. F. Wilcox, "Graph theory and molecular orbitals. XII. Acyclic polyenes," *The Journal of Chemical Physics*, vol. 62, pp. 3399–3405, 1975.

[5] T. Došlić, B. Furtula, A. Graovac, I. Gutman, S. Moradi, and Z. Yarahmadi, "On vertex–degree–based molecular structure descriptors," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 66, pp. 613–626, 2011.

[6] I. Gutman and M. Goubko, "Trees with fixed number of pendent vertices with minimal first Zagreb index," *Bulletin of the International Mathematical Virtual Institute*, vol. 3, pp. 161–164, 2013.

[7] M. Goubko, "Minimizing degree-based toplogical indices for trees with given number of pendent vertices," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 71, pp. 33–46, 2014.

[8] H. Lin, "On segments, vertices of degree two and the first Zagreb index of trees," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 72, pp. 825–834, 2014.

[9] B. Borovićanin, "On the extremal Zagreb indices of trees with given number of segments or given number of branching vertices," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 74, no. 1, pp. 57–79, 2015.

[10] B. Borovićanin, K. C. Das, B. Furtula, and I. Gutman, "Bounds for Zagreb indices," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 78, pp. 17–100, 2017.

[11] B. Borovićanin, K. C. Das, B. Furtula, and I. Gutman, "Zagreb indices: bounds and extremal graphs," in *Bounds in Chemical Graph Theory Basics*, I. Gutman, B. Furtula, K. C. Das, E. Milovanovi, and I. Milovanović, Eds., pp. 67–153, Univ. Kragujevac, Kragujevac, 2017.

[12] K. C. Das, A. Yurttas, M. Togan, A. S. Çevik, and I. N. Çangül, "The multiplicative Zagreb indices of graph operations," *Journal of Inequalities and Applications*, vol. 90, 2013.

[13] K. C. Das, N. Akgüneş, M. Togan, A. Yurttas, A. S. Çevik, and I. N. Çangül, "On the first Zagreb index and multiplicative Zagreb coindices of graphs," *Analele Stiintifice Ale Universitatii Ovidius Constanta-Seria Matematica*, vol. 24, no. 1, pp. 153–176, 2016.

[14] A. R. Bindusree, I. N. Çangül, V. Lokesha, and A. S. Çevik, "Zagreb polynomials of three graph operators," *Univerzitet u Nišu*, vol. 30, no. 7, pp. 1979–1986, 2016.

[15] S. Aykaç, N. Akgüneş, and A. S. Çevik, "Analysis of Zagreb indices over zero-divisor graphs of commutative rings," *Asian-European Journal of Mathematics*, vol. 12, no. 6, 2019.

[16] B. Borovićanin and T. A. Lampert, "On the maximum and minimum Zagreb indices of trees with a given number of vertices of maximum degree," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 74, no. 1, pp. 81–96, 2015.

[17] D. Stevanović and M. Milanič, "Improved inequality between Zagreb indices of trees," *Match-Communications in Mathematical and Computer Chemistry*, vol. 68, no. 1, pp. 147–156, 2012.

[18] D. Vukičević and G. Popivoda, "Chemical trees with extremal values of Zagreb indices and coindices," *Iranian Journal of Mathematical Chemistry*, vol. 5, pp. 19–29, 2014.

[19] D. A. Mojdeh, M. Habibi, L. Badakhshian, and Y. Rao, "Zagreb indices of trees, unicyclic and bicyclic graphs with given (total) dominaion," *IEEE Access*, vol. 7, pp. 94143–94149, 2019.

[20] F. Zhan, Y. Qiao, and J. Cai, "Relations between the first Zagreb index and spectral moment of graphs," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 81, pp. 383–392, 2019.

[21] M. H. Liu and B. L. Liu, "The second Zagreb indices and Wiener polarity indices of trees with given degree sequences," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 67, pp. 439–450, 2012.

[22] M. Hanif, A. A. Bhatti, M. Javid, and E. Bonyah, "On the extremal trees for some bond incident degree indices with a fixed number of segments," *Journal of Chemistry*, vol. 2022, Article ID 4032709, 29 pages, 2022.

[23] R. Rasi, S. M. Sheikholeslami, and A. Behmaram, "An upper bound on the first Zagreb index in trees," *Iranian Journal of Mathematical Chemistry*, vol. 8, no. 1, pp. 71–82, 2017.

[24] M. Rizwan, A. A. Bhatti, M. Javaid, and F. Jarad, "Some bounds on bond incident degree indices with some parameters," *Mathematical Problems in Engineering*, vol. 2021, Article ID 8417486, 10 pages, 2021.

[25] M. Rizwan, A. A. Bhatti, M. Javaid, and E. Bonyah, "Extremal values of variable sum exdeg index for conjugated bicyclic graphs," *Journal of Chemistry*, vol. 2021, Article ID 4272208, 11 pages, 2021.

[26] S. Wang, C. Wang, L. Chen, and J. B. Liu, "On extremal multiplicative Zagreb indices of trees with given number of vertices of maximum degree," *Applications of Mathematics*, vol. 227, pp. 166–173, 2017.

[27] M. Azari and A. Iranmanesh, "Generalized Zagreb index of graphs," *Studia Universitatis Babes-Bolyai Chemia*, vol. 56, no. 3, pp. 59–70, 2011.

[28] V. R. Kulli, "The Gourava indices and coindices of graphs," *Annals of Pure and Applied Mathematics*, vol. 14, pp. 33–38, 2017.

[29] V. R. Kulli, "On hyper–Gourava indices and coindices," *International Journal of Mathematical Archive*, vol. 8, no. 12, pp. 116–120, 2017.

[30] M. H. Aftab, M. Rafaqat, M. Hussain, and T. Zia, "On the computation of some topological descriptors to find closed formulas for certain chemical graphs," *Journal of Chemistry*, vol. 2021, Article ID 5533619, 16 pages, 2021.

[31] B. Basavanagoud and S. Policepatil, "Chemical applicability of Gourava and hyper-Gourava indices," *Nanosystems: Physics, Chemistry, Mathematics*, vol. 12, no. 2, pp. 142–150, 2021.