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Bounds on Atom-Bond Connectivity and Zagreb Indices in Trees with a Given Metric Dimension

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Abstract

Let $G = (V, E)$ be a simple connected graph, where V and E denote the vertex and edge sets, respectively. The first Zagreb index is defined as $H_1(G) = \sum_{\nu \in V} \deg_G(\nu)^2$. Meanwhile, the second Zagreb index is given by $H_2(G) = \sum_{\nu_1\nu_2 \in E} \deg_G(\nu_1)\ \deg_G(\nu_2)$, where $\deg_G(\nu)$ represents the degree of vertex ν. Another notable degree-based invariant is the Atom-Bond Connectivity (ABC) index, introduced in chemical graph theory, and defined by:

$$ABC(G) = \sum_{\nu_1\nu_2 \in E} \sqrt{\frac{\deg_G(\nu_1) + \deg_G(\nu_2) - 2}{\deg_G(\nu_1)\ \deg_G(\nu_2)}}.$$

A fundamental graph parameter, the Metric Dimension (MetDim), refers to the minimum number of vertices in a resolving set that uniquely distinguishes all other vertices based on distances. In this work, we investigate the influence of MetDim on the Zagreb and ABC indices within the class of trees. Accordingly, we derive sharp bounds-both upper and lower for $H_1(\mathbb{T})$ and $H_2(\mathbb{T})$, and provide an upper bound for the $ABC(\mathbb{T})$ index. All are expressed in terms of the tree's order and its MetDim. Additionally, we recognize the extremal tree structures that attain these extreme values. Overall, these findings underscore the role of MetDim in shaping topological descriptors and contribute to both theoretical graph analysis and practical applications in molecular chemistry.

Keywords: ABC index; Zagreb indices; metric dimension; tree; chemical graph theory; extremal bounds.

1 Introduction

Graph theory has long served as a bridge between discrete mathematics and the molecular sciences, particularly through its applications in chemical graph theory. In computational chemistry, where the objective is to model and predict molecular properties without relying directly on quantum mechanical computations, molecular graphs provide a powerful abstraction. In such representations, atoms correspond to vertices, and chemical bonds to edges, often omitting hydrogen atoms for simplicity [16]. Within this framework, topological indices, quantitative measures derived from the structure of molecular graphs, are employed to correlate molecular structure with chemical, physical, and biological properties.

Among the earliest and most influential topological indices are the first and second Zagreb indices, denoted $H_1(G)$ and $H_2(G)$, respectively. Introduced by Gutman and Trinajstić [16], these indices capture degree-based connectivity patterns and are defined for a graph $G = (V, E)$, as follows:

$$H_1(G) = \sum_{\nu \in V(G)} \deg_G(\nu)^2, \tag{1}$$

$$H_2(G) = \sum_{\nu_1\nu_2 \in E(G)} \deg_G(\nu_1)\deg_G(\nu_2), \tag{2}$$

where $\deg_G(\nu)$ denotes the degree of vertex ν in G. These indices have been widely applied in QSAR/QSPR studies for predicting molecular stability, boiling points, and reactivity [25].

In an effort to improve the predictive power of topological descriptors, particularly with respect to molecular branching and steric effects, Estrada et al. [13] introduced the Atom-Bond Connectivity (ABC) index, defined as:

$$ABC(G) = \sum_{\nu_1\nu_2 \in E} \sqrt{\frac{\deg_G(\nu_1) + \deg_G(\nu_2) - 2}{\deg_G(\nu_1)\ \deg_G(\nu_2)}}. \tag{3}$$

This index has demonstrated strong correlations with thermodynamic and structural properties, and has since become an essential tool in chemical graph theory [14].

A substantial body of work has been devoted to characterizing extremal values and establishing bounds for the ABC and Zagreb indices in various graph classes. For trees, Furtula et al. [14] revealed that the star graph $\mathbb{S}_n$ attains the maximum ABC index, a result further explored in chemical tree structures of bounded degree [26]. Following this, Chen and Guo [8] extended ABC extremal studies to catacondensed hexagonal systems and reported that edge deletion reduces the ABC index. Further contributions have identified ABC extremal graphs among BFS trees [21], cactus graphs [4], and graphs with specific connectivity or chromatic constraints [9]. Most recently, Wu and Zhang [28], Das et al. [10], and Ali et al. [1] have deepened the analysis of structural conditions that maximize or minimize the ABC index in chemical graphs.

In parallel, extensive research has also been conducted on bounding the Zagreb indices under various structural constraints. Works, such as those by Li and Zhou [20] investigated graphs with vertex or edge connectivity at most k, establishing sharp upper and lower bounds for the Zagreb indices. Li and Zhou [19] analyzed bipartite graphs with fixed diameter, deriving sharp upper bounds for the Zagreb indices and characterizing extremal structures. Borovićanin [5] established sharp extremal bounds for Zagreb indices of trees constrained by segment counts or branching vertices, characterizing the corresponding extremal structures. Borovićanin and Furtula [6] provide sharp bounds for Zagreb indices in graphs characterized by connectivity, matching numbers, and domination parameters. Further studies by Pei and Pan [23], Jia and Wang [18], Mojdeh et al. [22], and Enteshari and Taeri [12] have extended these investigations to graphs with pendent vertices, cut vertices, and distance domination conditions. Furthermore, Dehgardi [11] recently applied Roman domination numbers to establish sharp lower bounds for Zagreb indices. More recently, Ali et al. [2] analyzed extremal upper and lower bounds of the ABC index $ABC(\mathbb{T})$ for trees constrained by a fixed Roman domination number, characterizing extremal structures. In addition, Ali et al. [3] established a sharp lower bound for the second Hyper-Zagreb index $\mathrm{HM}_2(G)$ of trees in terms of order and Roman domination number $\Gamma_R(G)$, revealing structural dependencies.

Despite this rich literature, a notable gap remains in the role of MetDim, a parameter that measures the minimum number of landmarks needed to uniquely identify every vertex in a graph using bounding degree-based topological indices, which has not been explored. Notably, the MetDim provides insights into the graph's resolving capabilities and has practical implications in areas such as network navigation and robot localization.

This work aims to address this gap by investigating the bounds on the Zagreb indices and the ABC index for trees in terms of their order and MetDim. Specifically, we establish upper and lower bounds for Zagreb indices, and an upper bound for the ABC index. Furthermore, we identify the extremal trees that attain these bounds, thereby contributing to both the mathematical theory of graph invariants and chemical graph modeling.

The notation employed throughout this paper is defined and summarized in Table 1.

Symbol	Description	Symbol	Description
G	A graph	$\mathtt{n}$	Order of the graph
$V(G)$ or V	Vertex set of G	$\mathbb{P}_\mathtt{n}$	Path graph of order $\mathtt{n}$
$E(G)$ or E	Edge set of G	$\mathbb{S}_\mathtt{n}$	Star graph of order $\mathtt{n}$
ν	A vertex of G	$\mathbb{T}_\mathtt{n}$ or $\mathbb{T}$	Tree of order $\mathtt{n}$
$\deg_G(\nu)$	Degree of the vertex ν	$N(\nu)$	Neighborhood of the vertex ν
$\dim(G)$	Metric dimension of G	$H_1(G)$	First Zagreb index
$H_2(G)$	Second Zagreb index	$ABC(G)$	Atom–Bond Connectivity index
$G \setminus \{\nu\}$	Graph obtained from G by deleting the vertex ν	$\Gamma_R(\mathbb{T})$ or Γ_R	Roman domination number of $\mathbb{T}$
$\mathbb{f}_{lb}$	Lower bound	$\mathbb{f}_{ub}$	Upper bound

Table 1: List of Symbols

2 Preliminary

In this section, we outline the essential definitions and previously established results from the literature that form the basis for our work. These preliminary concepts are fundamental for the formulation of our approach and for proving the main results in the following section.

We denote by $\mathbb{T}\backslash\{\nu_1, \nu_2, \ldots, \nu_\mathtt{n}\}$ the tree obtained from $\mathbb{T}$ after removing the vertices $\nu_1, \nu_2, \ldots, \nu_\mathtt{n}$. As customary, $\mathbb{P}_\mathtt{n}$ (see Figure 1) and $\mathbb{S}_\mathtt{n}$ (see Figure 2) represent the path and the star graph on $\mathtt{n}$ vertices, respectively.

Theorem 2.1. [15] Let $\mathbb{P}_\mathtt{n}$ be a path graph with $\mathtt{n} \geq 3$ vertices. Its first and second Zagreb indices

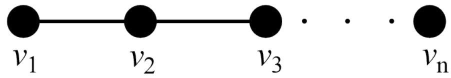

Figure 1: Path graph of order $\mathtt{n}(\mathbb{P}_{\mathtt{n}})$

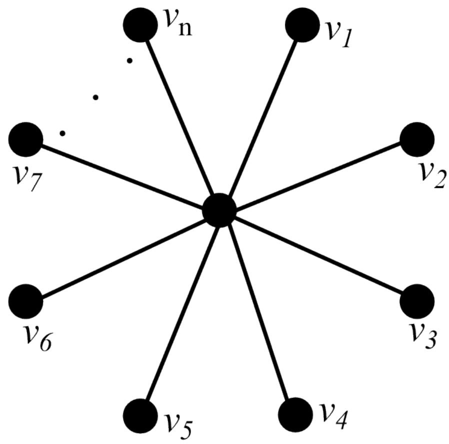

Figure 2: Star graph of order $\mathtt{n}$ $(\mathbb{S}_{\mathtt{n}})$

are defined by:

$$H_1(\mathbb{P}_{\mathtt{n}}) = 4\mathtt{n} - 6, \quad H_2(\mathbb{P}_{\mathtt{n}}) = 4\mathtt{n} - 8.$$

Theorem 2.2. [15] For $\mathbb{S}_{\mathtt{n}}$ with order $\mathtt{n} \geq 3$. Then,

$$H_1(\mathbb{S}_{\mathtt{n}}) = \mathtt{n}(\mathtt{n} - 1), \quad H_2(\mathbb{S}_{\mathtt{n}}) = (\mathtt{n} - 1)^2.$$

Definition 2.1. [27] The degree of a vertex ν in a graph G, denoted by $\deg_G(\nu)$, is the number of edges incident to ν. In a simple undirected graph, this is equal to the number of vertices adjacent to ν. Meanwhile, the open neighborhood of a vertex ν_1 in a graph G, denoted by $N(\nu_1)$, is the set of all vertices adjacent to ν_1, excluding ν_1 itself:

$$N(\nu) = \{\nu \in V(G) \mid \nu\nu_1 \in E(G)\}.$$

Definition 2.2. [27] A leaf in a graph is a vertex that has degree one; that is, it is connected to exactly one other vertex. In a tree $\mathbb{T}$, the diameter, denoted by d, refers to the longest distance between any pair of leaves. Moreover, a path $\mathbb{P}_{d+1} = \{\nu_1, \nu_2, \ldots, \nu_{d+1}\}$ in $\mathbb{T}$ is referred to as a diameter path if the distance between the endpoints ν_1 and ν_{d+1} is equal to d, indicating that it spans the full diameter of the tree.

Definition 2.3. [17, 24] Let $G = (V, E)$ represent a connected graph. A subset $\mathbb{W} \subseteq V(G)$ is termed a resolving set if, for every pair of distinct vertices $\nu_1, \nu_2 \in V(G)$, there exists at least one vertex $\omega \in \mathbb{W}$ such that the distances from ν_1 and ν_2 to ω are different, that is, $d(\nu_1, \omega) \neq d(\nu_2, \omega)$. Here, $d(\nu_i, \omega)$ denotes the shortest path length between vertex ν_i and ω. The MetDim of the graph G, denoted by $\dim(G)$, is defined as the smallest number of vertices in such a resolving set.

Theorem 2.3. [7] Let G be a graph. Then $\dim(G) = 1 \iff G$ is a path $\mathbb{P}_{\mathtt{n}}$.

Theorem 2.4. [7] Suppose that $\mathbb{S}_{\mathtt{n}}$ with $\mathtt{n} \geq 4$ vertices. Then $\dim(\mathbb{S}_{\mathtt{n}}) = \mathtt{n} - 2$.

Theorem 2.5. [14] If $\mathbb{S}_{\mathtt{n}}$ of order $\mathtt{n}$, then

$$ABC(\mathbb{S}_{\mathtt{n}}) = \sqrt{\mathtt{n} - 2}\,\sqrt{\mathtt{n} - 1}.$$

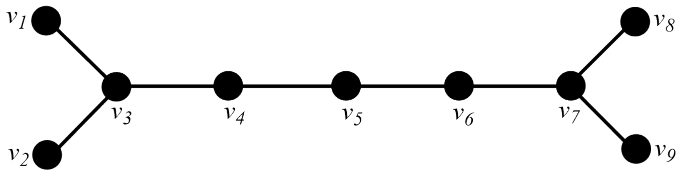

Figure 3: A tree of order nine

Consider the graph $\mathbb{T}$ displayed in Figure 3, whose vertex set is $\{\nu_1, \dots, \nu_9\}$. We examine two subsets of vertices, namely $\mathbb{W}_1 = \{\nu_1, \nu_2\}$ and $\mathbb{W}_2 = \{\nu_1, \nu_8\}$, and their corresponding metric representations listed in Tables 2 and 3. From Table 2, the equality $r(\nu_8 \mid \mathbb{W}_1) = r(\nu_9 \mid \mathbb{W}_1)$ indicates that $\mathbb{W}_1$ does not distinguish all vertices of $\mathbb{T}$ and hence is not a resolving set. In contrast, Table 3 demonstrates that all metric representations with respect to $\mathbb{W}_2$ are pairwise distinct, implying that $\mathbb{W}_2$ resolves the graph. Since $\mathbb{T}$ is not isomorphic to a path, no resolving set of cardinality one exists by Theorem 2.3. Furthermore, since $\mathbb{W}_2$ has minimum size among all resolving sets, we conclude that $\dim(\mathbb{T}) = 2$.

For the tree graph presented in Figure 3, we demonstrate the computation of the Zagreb indices and the ABC index. Using Equation 1, the vertex degrees are $d(\nu_1) = d(\nu_2) = d(\nu_8) = d(\nu_9) = 1$, $d(\nu_3) = d(\nu_7) = 3$, and $d(\nu_4) = d(\nu_5) = d(\nu_6) = 2$; hence, the first Zagreb index is $H_1(\mathbb{T}) = 4(1^2) + 2(3^2) + 3(2^2) = 34$. Using Equation 2, the second Zagreb index is $H_2(\mathbb{T}) = 1 \cdot 3 + 1 \cdot 3 + 3 \cdot 2 + 2 \cdot 2 + 2 \cdot 2 + 2 \cdot 3 + 3 \cdot 1 + 3 \cdot 1 = 32$. Similarly, by applying Equation 3, the ABC index of $\mathbb{T}$ is obtained as $ABC(\mathbb{T}) = 6.0944$.

ν_i	$r(\nu_i \mid \mathbb{W}_1)$	ν_i	$r(\nu_i \mid \mathbb{W}_1)$
ν_1	(0,2)	ν_6	$(4,4)$
ν_2	$(2,0)$	ν_7	$(5,5)$
ν_3	$(1,1)$	ν_8	$(6,6)$
ν_4	$(2,2)$	ν_9	$(6,6)$
ν_5	$(3,3)$		

Table 2: Vertex representations with respect to $\mathbb{W}_1$

ν_i	$r(\nu_i \mid \mathbb{W}_2)$	ν_i	$r(\nu_i \mid \mathbb{W}_2)$
ν_1	$(0,6)$	ν_6	$(4,2)$
ν_2	$(2,6)$	ν_7	$(5,1)$
ν_3	$(1,5)$	ν_8	$(6,0)$
ν_4	$(2,4)$	ν_9	$(6,2)$
ν_5	$(3,3)$		

Table 3: Vertex representations with respect to $\mathbb{W}_2$

3 Upper Bound on ABC index in Terms of Order and MetDim

An extensive survey presented in [14] explores the established bounds of the ABC index across various fundamental graph classes. In particular, within all trees having order $\mathtt{n}$, the star graph $\mathbb{S}_{\mathtt{n}}$ is known to attain the maximum ABC index. Building upon these findings, this section establishes new extremal values for the ABC index in trees, incorporating both the order and the MetDim as key structural parameters. Specifically, we define $\mathbb{f}_{ub}(\mathtt{n}, \dim(\mathbb{T}))$ as the sharp upper bound, which is rigorously derived and formally proven in Theorem 3.1.

Lemma 3.1. Let the function $F_1(\alpha)$ be defined as:

$$F_1(\alpha) = (\alpha - 1)\sqrt{\frac{\alpha - 1}{\alpha}} - (\alpha - 2)\sqrt{\frac{\alpha - 2}{\alpha - 1}},$$

for $\alpha \geq 3$. Then $F_1(\alpha)$ is positive and monotonically increasing.

Proof. Define
$$G(\alpha) = (\alpha - 1)\sqrt{\frac{\alpha - 1}{\alpha}}, \quad \alpha \geq 3.$$
Then, we can express
$$F_1(\alpha) = G(\alpha) - G(\alpha - 1).$$
Note that $G(\alpha) > 0$ for all $\alpha \geq 3$ since both $\alpha - 1$ and the square root term are positive.

Subsequently, we compute the derivative of $G(\alpha)$. Let
$$G(\alpha) = (\alpha - 1)\left(\frac{\alpha - 1}{\alpha}\right)^{1/2}.$$
Using the product and chain rules, we obtain:
$$G'(\alpha) = \sqrt{\frac{\alpha - 1}{\alpha}} + (\alpha - 1) \cdot \frac{1}{2}\left(\frac{\alpha - 1}{\alpha}\right)^{-1/2} \cdot \frac{\alpha - (\alpha - 1)}{\alpha^2}.$$
Simplifying,
$$G'(\alpha) = \sqrt{\frac{\alpha - 1}{\alpha}} + (\alpha - 1) \cdot \frac{1}{2}\left(\frac{\alpha}{\alpha - 1}\right)^{1/2} \cdot \frac{1}{\alpha^2}.$$
$$G'(\alpha) = \frac{\sqrt{\alpha - 1}}{\sqrt{\alpha}} + \frac{\alpha - 1}{2\alpha^2}\frac{\sqrt{\alpha}}{\sqrt{\alpha - 1}} = \frac{\sqrt{\alpha - 1}}{\sqrt{\alpha}} + \frac{\sqrt{\alpha - 1}}{2\alpha\sqrt{\alpha}}.$$
Combining terms offers
$$G'(\alpha) = \frac{\sqrt{\alpha - 1}}{\sqrt{\alpha}}\left(1 + \frac{1}{2\alpha}\right) = \frac{\sqrt{\alpha - 1}}{\sqrt{\alpha}} \cdot \frac{2\alpha + 1}{2\alpha}.$$
Since $\alpha \geq 3$, it follows that $G'(\alpha) > 0$. Therefore, $G(\alpha)$ is a strictly increasing function on $[3, \infty)$.

Finally, since $F_1(\alpha) = G(\alpha) - G(\alpha - 1)$ and $G(\alpha)$ is strictly increasing, it follows that
$$F_1(\alpha) > 0 \quad \text{for all } \alpha \geq 3,$$
and
$$F_1(\alpha + 1) - F_1(\alpha) = \big(G(\alpha + 1) - G(\alpha)\big) - \big(G(\alpha) - G(\alpha - 1)\big) > 0.$$
This is attributed to the fact that the increments of a strictly increasing function are themselves increasing. Hence, $F_1(\alpha)$ is positive and monotonically increasing for $\alpha \geq 3$. □

Lemma 3.2. Let
$$F_2(\alpha, \beta) = \sqrt{\frac{\alpha + \beta - 2}{\alpha\beta}} - \sqrt{\frac{\alpha + \beta - 3}{(\alpha - 1)\beta}},$$
for $\alpha \geq 3$ and $\beta \geq 2$. Then, $F_2(\alpha, \beta) \leq 0$ for all $\alpha \geq 3, \beta \geq 2$, whereas $F_2(\alpha, \beta) < 0$ when $\beta > 2$. For fixed $\beta \geq 2$ the function $\alpha \mapsto F_2(\alpha, \beta)$ is nondecreasing on $[3, \infty)$, and it is strictly increasing when $\beta > 2$.

Proof. Set
$$u(\alpha, \beta) = \sqrt{\frac{\alpha + \beta - 2}{\alpha\beta}}, \qquad v(\alpha, \beta) = \sqrt{\frac{\alpha + \beta - 3}{(\alpha - 1)\beta}}.$$

Both u and v are positive for the stated ranges of α, β. We first present $u \leq v$, which is equivalent to $u^2 \leq v^2$. Indeed,

$$\frac{\alpha+\beta-2}{\alpha\beta} \leq \frac{\alpha+\beta-3}{(\alpha-1)\beta},$$

if and only if

$$(\alpha+\beta-2)(\alpha-1) \leq (\alpha+\beta-3)\alpha.$$

Expanding both sides and simplifying yields

$$(\alpha+\beta-3)\alpha - (\alpha+\beta-2)(\alpha-1) = \beta-2 \geq 0.$$

This indicates that the displayed inequality holds. Hence, $u \leq v$, which implies

$$F_2(\alpha,\beta) = u - v \leq 0,$$

with equality precisely when $\beta = 2$ (in that case the two square-root terms coincide). For $\beta > 2$ the last displayed inequality is strict; thus, $F_2(\alpha,\beta) < 0$.

Next, we demonstrate monotonicity in α. Differentiate F_2 with respect to α. Computing $\partial u/\partial\alpha$ and $\partial v/\partial\alpha$ by the chain and product rules yields

$$\frac{\partial u}{\partial \alpha} = -\frac{\beta-2}{2\alpha^2\beta}\cdot\frac{1}{\sqrt{\dfrac{\alpha+\beta-2}{\alpha\beta}}}, \qquad \frac{\partial v}{\partial \alpha} = -\frac{\beta-2}{2(\alpha-1)^2\beta}\cdot\frac{1}{\sqrt{\dfrac{\alpha+\beta-3}{(\alpha-1)\beta}}}.$$

Therefore,

$$\frac{\partial F_2}{\partial \alpha} = \frac{\partial u}{\partial \alpha} - \frac{\partial v}{\partial \alpha} = -\frac{\beta-2}{2\beta}\left(\frac{1}{\alpha^2\sqrt{\dfrac{\alpha+\beta-2}{\alpha\beta}}} - \frac{1}{(\alpha-1)^2\sqrt{\dfrac{\alpha+\beta-3}{(\alpha-1)\beta}}}\right).$$

If $\beta = 2$ the prefactor $\beta - 2$ vanishes and hence $\partial F_2/\partial\alpha = 0$ (so F_2 is constant in α, consistent with the equality case above). Assume $\beta > 2$. Then $\beta - 2 > 0$ and the sign of $\partial F_2/\partial\alpha$ is the opposite of the sign of

$$T(\alpha,\beta) := \frac{1}{\alpha^2\sqrt{\dfrac{\alpha+\beta-2}{\alpha\beta}}} - \frac{1}{(\alpha-1)^2\sqrt{\dfrac{\alpha+\beta-3}{(\alpha-1)\beta}}}.$$

We will demonstrate $T(\alpha,\beta) < 0$ for $\alpha \geq 3,\ \beta > 2$.

The inequality $T < 0$ is equivalent (after multiplying by the positive quantity $\alpha^2(\alpha-1)^2$ $\sqrt{\dfrac{\alpha+\beta-2}{\alpha\beta}}\sqrt{\dfrac{\alpha+\beta-3}{(\alpha-1)\beta}}$) to

$$(\alpha-1)^2\sqrt{\frac{\alpha+\beta-3}{(\alpha-1)\beta}} < \alpha^2\sqrt{\frac{\alpha+\beta-2}{\alpha\beta}}.$$

Squaring both sides (all terms are positive) yields the equivalent inequality

$$(\alpha-1)^4\frac{\alpha+\beta-3}{(\alpha-1)\beta} < \alpha^4\frac{\alpha+\beta-2}{\alpha\beta},$$

which simplifies to

$$(\alpha-1)^3(\alpha+\beta-3) < \alpha^3(\alpha+\beta-2).$$

Now, observe

$$\begin{aligned}\alpha^3(\alpha+\beta-2)-(\alpha-1)^3(\alpha+\beta-3) &= \left[\alpha^3(\alpha+\beta-2)-\alpha^3(\alpha+\beta-3)\right] \\ &\quad+\left[\alpha^3(\alpha+\beta-3)-(\alpha-1)^3(\alpha+\beta-3)\right], \\ &= \alpha^3+(\alpha+\beta-3)\big(\alpha^3-(\alpha-1)^3\big).\end{aligned}$$

Since $\alpha^3-(\alpha-1)^3 = 3\alpha^2-3\alpha+1 > 0$ for $\alpha \geq 3$ and $\alpha^3 > 0$, the right-hand side is positive. Hence,

$$(\alpha-1)^3(\alpha+\beta-3) < \alpha^3(\alpha+\beta-2),$$

Indicating that the squared inequality holds, and therefore $T(\alpha,\beta) < 0$. Consequently, the factor in parentheses above is negative, and with the prefactor $-(\beta-2)/(2\beta) < 0$, we obtain:

$$\frac{\partial F_2}{\partial \alpha}(\alpha,\beta) > 0 \qquad \text{for } \alpha \geq 3,\ \beta > 2.$$

This suggests that F_2 is strictly increasing in α when $\beta > 2$ and nondecreasing when $\beta = 2$. Correspondingly, combining these results finishes the proof. □

Lemma 3.3. Let the function $F_3(\alpha,\beta)$ be defined as:

$$F_3(\alpha,\beta) = F_1(\alpha)+F_2(\alpha,\beta).$$

For all $\alpha \geq 3$ and $\beta \geq 2$,

$$F_3(\alpha,\beta) > \frac{\sqrt{5}}{2\sqrt{2}}.$$

Equivalently, the global minimum of F_3 on the domain $\{(\alpha,\beta) : \alpha \geq 3, \beta \geq 2\}$ is strictly greater than $\frac{\sqrt{5}}{2\sqrt{2}}$.

Proof. By Lemma 3.1, $\alpha \mapsto F_1(\alpha)$ is strictly increasing for $\alpha \geq 3$. By Lemma 3.2, for each fixed $\beta \geq 2$ the map $\alpha \mapsto F_2(\alpha,\beta)$ is nondecreasing on $[3,\infty)$, and for each fixed $\alpha \geq 3$ the map $\beta \mapsto F_2(\alpha,\beta)$ is nonincreasing on $[2,\infty)$. Since $F_3(\alpha,\beta) = F_1(\alpha)+F_2(\alpha,\beta)$, these facts imply:

For every fixed $\beta \geq 2 : \inf_{\alpha \geq 3} F_3(\alpha,\beta) = F_3(3,\beta)$, and for every fixed $\alpha \geq 3 : \inf_{\beta \geq 2} F_3(\alpha,\beta) = \lim_{\beta\to\infty} F_3(\alpha,\beta)$.

Combining the two monotonicity conclusions implies that the global infimum of F_3 on the rectangle $\{(\alpha,\beta) : \alpha \geq 3,\ \beta \geq 2\}$ is attained at the boundary point with the smallest α and largest β, i.e.,

$$\inf_{\alpha\geq 3,\ \beta\geq 2} F_3(\alpha,\beta) = \lim_{\beta\to\infty} F_3(3,\beta).$$

We now evaluate this limit. From the definitions

$$F_1(3) = 2\sqrt{\frac{2}{3}}-\frac{1}{\sqrt{2}}, \qquad \lim_{\beta\to\infty} F_2(3,\beta) = \sqrt{\frac{1}{3}}-\frac{1}{\sqrt{2}}.$$

Hence,

$$\inf_{\alpha\geq 3,\ \beta\geq 2} F_3(\alpha,\beta) = F_1(3)+\lim_{\beta\to\infty} F_2(3,\beta) = 2\sqrt{\tfrac{2}{3}}+\sqrt{\tfrac{1}{3}}-\frac{2}{\sqrt{2}}.$$

Set
$$L := 2\sqrt{\tfrac{2}{3}} + \sqrt{\tfrac{1}{3}} - \frac{2}{\sqrt{2}}.$$
A direct numerical evaluation (or straightforward algebraic comparison) offers
$$L \approx 0.79612987 \quad \text{and} \quad \frac{\sqrt{5}}{2\sqrt{2}} = \sqrt{\frac{5}{8}} \approx 0.79056942,$$
which indicates that $L > \frac{\sqrt{5}}{2\sqrt{2}}$. Therefore, the global minimum of F_3 on $\{\alpha \geq 3, \beta \geq 2\}$ exceeds $\frac{\sqrt{5}}{2\sqrt{2}}$. It follows that there are no admissible (α, β) for which
$$F_3(\alpha, \beta) < \frac{\sqrt{5}}{2\sqrt{2}}.$$

This completes the proof. □

Theorem 3.1. Let $\mathbb{T}$ be a tree of order $\mathtt{n}$ and $\dim(\mathbb{T})$ is MetDim of $\mathbb{T}$. Then,
$$ABC(\mathbb{T}) \leq \sqrt{\mathtt{n}^2 - 3\mathtt{n} + 2} + (\mathtt{n} - 2 - \dim(\mathbb{T}))\left(\frac{4}{5} - \frac{2}{\sqrt{5}}\right).$$

Proof. Suppose that $\mathbb{f}_{ub}(\mathtt{n}, \dim(\mathbb{T})) = \sqrt{\mathtt{n}^2 - 3\mathtt{n} + 2} + (\mathtt{n} - 2 - \dim(\mathbb{T}))\left(\frac{4}{5} - \frac{2}{\sqrt{5}}\right)$ is a function. We claim that $ABC(\mathbb{T}) \leq \mathbb{f}_{ub}(\mathtt{n},\ \dim(\mathbb{T}))$, and prove this assertion by mathematical induction on $\mathtt{n}$. For the base case $\mathtt{n} = 4$, the two possible non-isomorphic graphs of order 4 are the path graph $\mathbb{P}_4$ and the star graph $\mathbb{S}_4$. A direct computation verifies that $ABC(\mathbb{S}_4) = \mathbb{f}_{ub}(\mathtt{n},\ \dim(\mathbb{T}))$ and $ABC(\mathbb{P}_4) < \mathbb{f}_{ub}(\mathtt{n},\ \dim(\mathbb{T}))$, establishing the base case. Now, assuming the inequality holds for all trees of order $\mathtt{n} - 1$, we proceed to demonstrate that it remains valid when the order of $\mathbb{T}$ is $\mathtt{n}$. Correspondingly, we discuss three cases.

Case 1: Suppose that $\mathbb{T}$ has maximum degree $\Delta = \mathtt{n} - 1$. This implies that $\mathbb{T} \cong \mathbb{S}_\mathtt{n}$. Using Theorems 2.1 and 2.4, we obtain the following:
$$\begin{aligned}
ABC(\mathbb{S}_\mathtt{n}) &= \sqrt{\mathtt{n} - 2}\sqrt{\mathtt{n} - 1}, \\
&= \sqrt{\mathtt{n} - 2}\sqrt{\mathtt{n} - 1} + (\mathtt{n} - 2 - \dim(\mathbb{T}))\left(\frac{4}{5} - \frac{2}{\sqrt{5}}\right), \\
&= \sqrt{\mathtt{n}^2 - 3\mathtt{n} + 2} + (\mathtt{n} - 2 - \dim(\mathbb{T}))\left(\frac{4}{5} - \frac{2}{\sqrt{5}}\right), \\
&= \mathbb{f}_{ub}(\mathtt{n}, \dim(\mathbb{S}_\mathtt{n})).
\end{aligned}$$

Notably, Case 1 demonstrates that when $\mathbb{T} \cong \mathbb{S}_\mathtt{n}$, we have $ABC(\mathbb{S}_\mathtt{n}) = \mathbb{f}_{ub}(\mathtt{n}, \dim(\mathbb{S}_\mathtt{n}))$. Therefore, $\mathbb{S}_\mathtt{n}$ is the tree that maximizes the ABC index.

Case 2: Consider the case where $\mathbb{T}$ has maximum degree $3 \leq \Delta < \mathtt{n} - 1$. Let $\mathbb{P}_{d+1} = \{\nu_1, \nu_2, \ldots, \nu_{d+1}\}$ represent a path of diameter in $\mathbb{T}$, and assume that $\xi_\mathbb{T}(\nu_2) \geq 2$.

Case 2.1: Suppose that $\xi_\mathbb{T}(\nu_2) = 3$ and $\xi_\mathbb{T}(\nu_3) = \Upsilon \geq 3$. The neighborhood of ν_2 is $N(\nu_2) = \{\nu_1, \nu_3, \nu\}$, where $\xi_\mathbb{T}(\nu) = 1$. Define the modified tree $\mathbb{T}' = \mathbb{T} \setminus \{\nu_1\}$. In this case, the value of $\dim(\mathbb{T})$ remains invariant, implying that $\dim(\mathbb{T}') = \dim(\mathbb{T})$. Consequently, we obtain:

$$\begin{aligned}
ABC(\mathbb{T}) =& ABC(\mathbb{T}') + \sqrt{\frac{\Upsilon+1}{3\Upsilon}} + 2\left(\sqrt{\frac{2}{3}} - \sqrt{\frac{1}{2}}\right),\\
\leq & \sqrt{(\mathtt{n}-1)^2 - 3(\mathtt{n}-1)+2} + (\mathtt{n}-3-\dim(\mathbb{T}'))\left(\frac{4}{5} - \frac{2}{\sqrt{5}}\right) + \sqrt{\frac{\Upsilon+1}{3\Upsilon}} + 2\left(\sqrt{\frac{2}{3}} - \sqrt{\frac{1}{2}}\right),\\
=& \mathbb{f}_{ub}(\mathtt{n},\ \dim(\mathbb{T})) + \sqrt{(\mathtt{n}-1)^2 - 3(\mathtt{n}-1)+2} - \sqrt{\mathtt{n}^2 - 3\mathtt{n}+2} + \sqrt{\frac{\Upsilon+1}{3\Upsilon}} - \left(\frac{4}{5} - \frac{2}{\sqrt{5}}\right)\\
& + 2\left(\sqrt{\frac{2}{3}} - \sqrt{\frac{1}{2}}\right).
\end{aligned}$$

Suppose that the function $f(\mathtt{n},\Upsilon)$ is defined as:

$$f(\mathtt{n},\Upsilon) = \sqrt{(\mathtt{n}-1)^2 - 3(\mathtt{n}-1)+2} - \sqrt{\mathtt{n}^2 - 3\mathtt{n}+2} + \sqrt{\frac{\Upsilon+1}{3\Upsilon}} - \left(\frac{4}{5} - \frac{2}{\sqrt{5}}\right) + 2\left(\sqrt{\frac{2}{3}} - \sqrt{\frac{1}{2}}\right).$$

We claim that $f(\mathtt{n},\Upsilon)$ is a negative function. To establish this, we decompose $f(\mathtt{n},\Upsilon)$ into two separate functions:

$$\begin{aligned}
f_1(\mathtt{n}) &= \sqrt{(\mathtt{n}-1)^2 - 3(\mathtt{n}-1)+2} - \sqrt{\mathtt{n}^2 - 3\mathtt{n}+2},\\
f_2(\Upsilon) &= \sqrt{\frac{\Upsilon+1}{3\Upsilon}} - \left(\frac{4}{5} - \frac{2}{\sqrt{5}}\right) + 2\left(\sqrt{\frac{2}{3}} - \sqrt{\frac{1}{2}}\right).
\end{aligned}$$

First, we analyze $f_1(\mathtt{n})$. By rewriting it in terms of the function $f_{1'}(\mathtt{n}) = \sqrt{\mathtt{n}^2 - 3\mathtt{n}+2}$, we compute its derivative:

$$\frac{d}{dn} f_{1'}(\mathtt{n}) = \frac{2\mathtt{n}-3}{2\sqrt{\mathtt{n}^2 - 3\mathtt{n}+2}}.$$

Since this derivative is positive for $\mathtt{n} \geq 5$, it follows that $f_{1'}(\mathtt{n})$ is an increasing function. As a result, $f_1(\mathtt{n})$ is negative and bounded within the interval $(-1.015, -1)$. Following this, we consider $f_2(\Upsilon)$. Computing its derivative, we obtain:

$$\frac{d}{d\Upsilon} f_2(\Upsilon) = -\frac{1}{2\sqrt{3}\Upsilon\mathtt{n}^2\sqrt{\frac{\Upsilon+1}{\Upsilon}}}.$$

Since this derivative is negative, $f_2(\Upsilon)$ is a decreasing function and is bounded within the interval $(0.89, 0.98)$. Thus, summing both components, we conclude that $f(\mathtt{n},\Upsilon) = f_1(\mathtt{n}) + f_2(\Upsilon)$ is negative, as required. Therefore,

$$ABC(\mathbb{T}) = \mathbb{f}_{ub}(\mathtt{n},\ \dim(\mathbb{T})) + f(\mathtt{n},\Upsilon) < \mathbb{f}_{ub}(\mathtt{n},\dim(\mathbb{T})).$$

Case 2.1.1: Suppose that $\xi_{\mathbb{T}}(\nu_3) = 2$. Define the modified tree $\mathbb{T}' = \mathbb{T} \setminus \{\nu_1, \nu\}$. In this case, $\dim(\mathbb{T})$ is still invariant, implying that $\dim(\mathbb{T}') = \dim(\mathbb{T})$. Consequently, we have:

$$\begin{aligned}
ABC(\mathbb{T}) =& ABC(\mathbb{T}') + 2\sqrt{\frac{2}{3}},\\
\leq & \sqrt{(\mathtt{n}-2)^2 - 3(\mathtt{n}-2)+2} + (\mathtt{n}-4-\dim(\mathbb{T}'))\left(\frac{4}{5} - \frac{2}{\sqrt{5}}\right) + 2\sqrt{\frac{2}{3}},\\
=& \mathbb{f}_{ub}(\mathtt{n},\ \dim(\mathbb{T})) + \sqrt{(\mathtt{n}-2)^2 - 3(\mathtt{n}-2)+2} - \sqrt{\mathtt{n}^2 - 3\mathtt{n}+2} - 2\left(\frac{4}{5} - \frac{2}{\sqrt{5}}\right) + 2\sqrt{\frac{2}{3}}.
\end{aligned}$$

Suppose that $f(\mathtt{n}) = \sqrt{(\mathtt{n}-2)^2 - 3(\mathtt{n}-2)+2} - \sqrt{\mathtt{n}^2 - 3\mathtt{n}+2} - 2\left(\frac{4}{5} - \frac{2}{\sqrt{5}}\right) + 2\sqrt{\frac{2}{3}}$, and $f(\mathtt{n})$ is negative function for $\mathtt{n} \geq 5$. Therefore,

$$ABC(\mathbb{T}) = \mathbb{f}_{ub}(\mathtt{n},\ \dim(\mathbb{T})) + f(\mathtt{n}) < \mathbb{f}_{ub}(\mathtt{n},\ \dim(\mathbb{T})).$$

Case 2.2: Assume that $\xi_{\mathbb{T}}(\nu_2) = \psi \geq 4$ and $\xi_{\mathbb{T}}(\nu_3) = \Upsilon$. The neighborhood of ν_2 is defined as $N(\nu_2) = \{\nu_1, \nu_3, z_1, \ldots, z_{\psi-2}\}$, where $\xi_{\mathbb{T}}(z_i) = 1$ and $1 \leq i \leq \psi - 2$. Now, let $T' = T \backslash \{\nu_1\}$ represent the modified tree. In this case, the value of $\dim(\mathbb{T})$ changed, indicating that $\dim(\mathbb{T}') = \dim(\mathbb{T}) - 1$. Thus, we obtain:

$$\begin{aligned}
ABC(\mathbb{T}) =& ABC(\mathbb{T}') + \frac{(\psi-1)^{\frac{3}{2}}}{\sqrt{\psi}} - \frac{(\psi-2)^{\frac{3}{2}}}{\sqrt{\psi-1}} + \sqrt{\frac{\psi+\Upsilon-2}{\psi l}} - \sqrt{\frac{\psi+\Upsilon-3}{(\psi-1)\Upsilon}},\\
\leq& \sqrt{(\mathtt{n}-1)^2 - 3(\mathtt{n}-1)+2} + (\mathtt{n}-3-\dim(\mathbb{T}'))\left(\frac{4}{5} - \frac{2}{\sqrt{5}}\right) + \frac{(\psi-1)^{\frac{3}{2}}}{\sqrt{\psi}} + \sqrt{\frac{\psi+\Upsilon-2}{\psi l}}\\
&- \frac{(\psi-2)^{\frac{3}{2}}}{\sqrt{\psi-1}} - \sqrt{\frac{\psi+\Upsilon-3}{(\psi-1)\Upsilon}},\\
=& \sqrt{(\mathtt{n}-1)^2 - 3(\mathtt{n}-1)+2} + (\mathtt{n}-3-(\dim(\mathbb{T}-1)))\left(\frac{4}{5} - \frac{2}{\sqrt{5}}\right) + \frac{(\psi-1)^{\frac{3}{2}}}{\sqrt{\psi}}\\
&+ \sqrt{\frac{\psi+\Upsilon-2}{\psi l}} - \frac{(\psi-2)^{\frac{3}{2}}}{\sqrt{\psi-1}} - \sqrt{\frac{\psi+\Upsilon-3}{(\psi-1)\Upsilon}},\\
=& \sqrt{(\mathtt{n}-1)^2 - 3(\mathtt{n}-1)+2} + (\mathtt{n}-2-\dim(\mathbb{T}))\left(\frac{4}{5} - \frac{2}{\sqrt{5}}\right) + \frac{(\psi-1)^{\frac{3}{2}}}{\sqrt{\psi}}\\
&+ \sqrt{\frac{\psi+\Upsilon-2}{\psi l}} - \frac{(\psi-2)^{\frac{3}{2}}}{\sqrt{\psi-1}} - \sqrt{\frac{\psi+\Upsilon-3}{(\psi-1)\Upsilon}},\\
=& \mathbb{f}_{ub}(\mathtt{n},\ \dim(\mathbb{T})) - \sqrt{\mathtt{n}^2 - 3\mathtt{n}+2} + \sqrt{(\mathtt{n}-1)^2 - 3(\mathtt{n}-1)+2} + (\psi-1)\sqrt{\frac{\psi-1}{\psi}}\\
&+ \sqrt{\frac{\psi+\Upsilon-2}{\psi l}} - (\psi-2)\sqrt{\frac{\psi-2}{\psi-1}} - \sqrt{\frac{\psi+\Upsilon-3}{(\psi-1)\Upsilon}}.
\end{aligned}$$

Consider the function $f(\mathtt{n}) = -\sqrt{\mathtt{n}^2 - 3\mathtt{n}+2} + \sqrt{(\mathtt{n}-1)^2 - 3(\mathtt{n}-1)+2}$ and define $g(\psi, \Upsilon) = (\psi-1)\sqrt{\frac{\psi-1}{\psi}} + \sqrt{\frac{\psi+\Upsilon-2}{\psi\Upsilon}} - (\psi-2)\sqrt{\frac{\psi-2}{\psi-1}} - \sqrt{\frac{\psi+\Upsilon-3}{(\psi-1)\Upsilon}}$. From the result established in Case 2.1, we have $-1.015 < f(\mathtt{n}) < -1$. Additionally, by applying Lemma 3.3, it follows that $0.796 < g(\psi, \Upsilon) < 1$. Since $f(\mathtt{n})$ is negative and $g(\psi, \Upsilon)$ remains positive, their sum $w(\mathtt{n}, \psi, \Upsilon) = f(\mathtt{n}) + g(\psi, \Upsilon)$ is negative. Therefore, the function $w(\mathtt{n}, \psi, \Upsilon)$ is strictly less than zero. Hence,

$$ABC(\mathbb{T}) = \mathbb{f}_{ub}(\mathtt{n},\ \dim(\mathbb{T})) + w(\mathtt{n}, \psi, \Upsilon) < \mathbb{f}_{ub}(\mathtt{n},\ \dim(\mathbb{T})).$$

Case 2.3: Suppose that $\xi_{\mathbb{T}}(\nu_2) = 2$ and $\xi_{\mathbb{T}}(\nu_3) \geq 2$.

Case 2.3.1: Consider the case where $\xi_{\mathbb{T}}(\nu_3) = \psi$, where $\psi = \{2, 3\}$, with $N(\nu_3) = \{\nu_2, \nu_4, \nu_k\}$, $k \leq \psi - 2$, $\xi_{\mathbb{T}}(\nu_k) = 1$, and $\xi_{\mathbb{T}}(\nu_4) = \Upsilon$. Define $\mathbb{T}' = \mathbb{T} \setminus \{\nu_1, \nu_2\}$. Under these conditions, $\dim(\mathbb{T}') = \dim(\mathbb{T})$. Therefore,

$$
\begin{aligned}
ABC(\mathbb{T}) =& ABC(\mathbb{T}') + \sqrt{\frac{\psi-1}{\psi}} - \sqrt{\frac{\psi+\Upsilon-3}{(\psi-1)\Upsilon}} + \sqrt{\frac{\psi+\Upsilon-2}{\psi\Upsilon}} + \sqrt{\frac{1}{2}},\\
\leq& \sqrt{(\mathtt{n}-2)^2-3(\mathtt{n}-2)+2} + (\mathtt{n}-4-\dim(\mathbb{T}'))\left(\frac{4}{5}-\frac{2}{\sqrt{5}}\right) + \sqrt{\frac{\psi-1}{\psi}} + \sqrt{\frac{\psi+\Upsilon-2}{\psi\Upsilon}}\\
&- \sqrt{\frac{\psi+\Upsilon-3}{(\psi-1)\Upsilon}} + \sqrt{\frac{1}{2}},\\
=& \mathbb{f}_{ub}(\mathtt{n},\ \dim(\mathbb{T})) - \sqrt{\mathtt{n}^2-3\mathtt{n}+2} + \sqrt{(\mathtt{n}-2)^2-3(\mathtt{n}-2)+2} + \sqrt{\frac{\psi-1}{\psi}} + \sqrt{\frac{\psi+\Upsilon-2}{\psi\Upsilon}}\\
&- \sqrt{\frac{\psi+\Upsilon-3}{(\psi-1)\Upsilon}} + \sqrt{\frac{1}{2}} - 2\left(\frac{4}{5}-\frac{2}{\sqrt{5}}\right).
\end{aligned}
$$

Consider the functions $f(\mathtt{n}) = -\sqrt{\mathtt{n}^2-3\mathtt{n}+2} + \sqrt{(\mathtt{n}-2)^2-3(\mathtt{n}-2)+2}$ and $g(\psi,\Upsilon) = \sqrt{\frac{\psi+\Upsilon-2}{\psi\Upsilon}} - \sqrt{\frac{\psi+\Upsilon-3}{(\psi-1)\Upsilon}} + \sqrt{\frac{1}{2}} - 2\left(\frac{4}{5}-\frac{2}{\sqrt{5}}\right)$. It is straightforward to verify that $f(\mathtt{n})$ is a negative function, with values constrained within the interval $(-2.0226,-2)$ for $\mathtt{n}\geq 6$. Additionally, $g(\psi,\Upsilon)$ is a positive function, bounded within $(1.56, 1.72)$. Since their sum remains negative, it follows that $w(\mathtt{n},\psi,\Upsilon) = f(\mathtt{n}) + g(\psi,\Upsilon) < 0$. Consequently:

$$ABC(\mathbb{T}) = \mathbb{f}_{ub}(\mathtt{n},\ \dim(\mathbb{T})) + w(\mathtt{n},\psi,\Upsilon) < \mathbb{f}_{ub}(\mathtt{n},\ \dim(\mathbb{T})).$$

Case 2.3.2: Suppose that $\xi_{\mathbb{T}}(\nu_3) = \psi \geq 4$, where the neighborhood of ν_3 is given by $N(\nu_3) = \{\nu_2, \nu_4, \nu_1, \ldots, \nu_{\psi-2}\}$, and assume that $\xi_{\mathbb{T}}(\nu_{\psi-2}) = 1$ and $\xi_{\mathbb{T}}(\nu_4) = \Upsilon$. Define $T' = T \setminus \{\nu_1, \nu_2, \nu_1\}$. In this scenario, $\dim(\mathbb{T}') = \dim(\mathbb{T}) - 2$. Hence, we obtain:

$$
\begin{aligned}
ABC(\mathbb{T}) =& ABC(\mathbb{T}') + (\psi-2)\sqrt{\frac{\psi-1}{\psi}} - (\psi-3)\sqrt{\frac{\psi+1}{\psi-2}} + \sqrt{\frac{\psi+\Upsilon-2}{\psi\Upsilon}} - \sqrt{\frac{\psi+\Upsilon-4}{(\psi-2)\Upsilon}} + \sqrt{2},\\
\leq& \sqrt{(\mathtt{n}-3)^2-3(\mathtt{n}-3)+2} + (\mathtt{n}-3-2-\dim(\mathbb{T}'))\left(\frac{4}{5}-\frac{2}{\sqrt{5}}\right) + (\psi-2)\sqrt{\frac{\psi-1}{\psi}}\\
&+ \sqrt{\frac{\psi+\Upsilon-2}{\psi\Upsilon}} - (\psi-3)\sqrt{\frac{\psi+1}{\psi-2}} - \sqrt{\frac{\psi+\Upsilon-4}{(\psi-2)\Upsilon}} + \sqrt{2}.\\
=& \sqrt{(\mathtt{n}-3)^2-3(\mathtt{n}-3)+2} + (\mathtt{n}-3-2-(\dim(\mathbb{T}-2))\left(\frac{4}{5}-\frac{2}{\sqrt{5}}\right) + (\psi-2)\sqrt{\frac{\psi-1}{\psi}}\\
&+ \sqrt{\frac{\psi+\Upsilon-2}{\psi\Upsilon}} - (\psi-3)\sqrt{\frac{\psi+1}{\psi-2}} - \sqrt{\frac{\psi+\Upsilon-4}{(\psi-2)\Upsilon}} + \sqrt{2},
\end{aligned}
$$

$$=\sqrt{(\mathtt{n}-3)^2-3(\mathtt{n}-3)+2}+(\mathtt{n}-3-\dim(\mathbb{T}))\left(\frac{4}{5}-\frac{2}{\sqrt{5}}\right)+(\psi-2)\sqrt{\frac{\psi-1}{\psi}}$$
$$+\sqrt{\frac{\psi+\Upsilon-2}{\psi\Upsilon}}-(\psi-3)\sqrt{\frac{\psi+1}{\psi-2}}-\sqrt{\frac{\psi+\Upsilon-4}{(\psi-2)\Upsilon}}+\sqrt{2},$$
$$=\mathbb{f}_{ub}(\mathtt{n},\ \dim(\mathbb{T}))-\sqrt{\mathtt{n}^2-3\mathtt{n}+2}+\sqrt{(\mathtt{n}-3)^2-3(\mathtt{n}-3)+2}+(\psi-2)\sqrt{\frac{\psi-1}{\psi}}$$
$$+\sqrt{\frac{\psi+\Upsilon-2}{\psi\Upsilon}}-(\psi-3)\sqrt{\frac{\psi+1}{\psi-2}}-\sqrt{\frac{\psi+\Upsilon-4}{(\psi-2)\Upsilon}}+\sqrt{2}-\left(\frac{4}{5}-\frac{2}{\sqrt{5}}\right).$$

Let $f(\mathtt{n})=-\sqrt{\mathtt{n}^2-3\mathtt{n}+2}+\sqrt{(\mathtt{n}-3)^2-3(\mathtt{n}-3)+2}$ and $g(\psi,\Upsilon)=(\psi-2)\sqrt{\frac{\psi-1}{\psi}}+\sqrt{\frac{\psi+\Upsilon-2}{\psi\Upsilon}}-(\psi-3)\sqrt{\frac{\psi+1}{\psi-2}}-\sqrt{\frac{\psi+\Upsilon-4}{(\psi-2)\Upsilon}}+\sqrt{2}-\left(\frac{4}{5}-\frac{2}{\sqrt{5}}\right)$. It is straightforward to verify that $f(\mathtt{n})$ is a negative function, with values restricted to the interval $(-3.05,-3)$ for $\mathtt{n}\geq 6$. Furthermore, $g(\psi,\Upsilon)$ is a positive function, bounded within $(0.50,1.66)$. Since their sum remains negative, it follows that $w(\mathtt{n},\psi,\Upsilon)=f(\mathtt{n})+g(\psi,\Upsilon)<0$. Thus:

$$ABC(\mathbb{T})=\mathbb{f}_{ub}(\mathtt{n},\ \dim(\mathbb{T}))+w(\mathtt{n},\psi,\Upsilon)<\mathbb{f}_{ub}(\mathtt{n},\ \dim(\mathbb{T})).$$

In other words, the theorem is proven. □

4 Bounds on Zagreb Indices in Terms of Order and MetDim

In this section, we establish bounds for the Zagreb indices of trees, expressed in terms of their order and MetDim. By exploring these relationships, we provide analytical insights into how structural parameters of a tree influence its corresponding Zagreb indices.

Theorem 4.1. Assume that $\mathbb{T}$ be a tree with order $\mathtt{n}$ and MetDim $\dim(\mathbb{T})$. Then, the inequality:

$$H_1(\mathbb{T})\geq 4\mathtt{n}+\dim(\mathbb{T})-7,$$

is satisfied.

Proof. $\mathbb{f}$ Assume that $\mathbb{f}_{lb}(\mathtt{n},\dim(\mathbb{T}))=4\mathtt{n}+\dim(\mathbb{T})-7$. We prove the claim by induction on $\mathtt{n}$. When $\mathtt{n}\geq 4$, Theorems 2.1 and 2.3 offer $H_1(\mathbb{P}_4)=10=\mathbb{f}_{lb}(4,1)$, and from Theorems 2.2 and 2.4, we have $H_1(\mathbb{S})=12\geq\mathbb{f}_{lb}(4,2)$. Now, assume the statement holds for all trees of $\mathtt{n}-1$ vertices. To prove the result of a tree of order $\mathtt{n}$, we shall consider the two following cases. **Case 1:** Suppose that we choose $\Delta(\mathbb{T})=2$, and in an obvious sense $\mathbb{T}\cong\mathbb{P}_{\mathtt{n}}$. From Theorem 2.1, we obtain $H_1(\mathbb{P}_{\mathtt{n}})$, and from Theorem 2.3, we deduce $\dim(\mathbb{P}_{\mathtt{n}})$.

$$\begin{aligned}H_1(\mathbb{P}_{\mathtt{n}})&=4\mathtt{n}-6,\\&=4\mathtt{n}+\dim(\mathbb{P}_{\mathtt{n}})-7,\\&=\mathbb{f}_{lb}(\mathtt{n},\ \dim(\mathbb{T})).\end{aligned}$$

In essence, equality occurs if $\mathbb{T}\cong\mathbb{P}_{\mathtt{n}}$. In response, we conclude that, in this case, $H_1(\mathbb{T})$ takes its minimum value.

Case 2: Let $\mathbb{P}_{d+1} = \{\nu_1, \nu_2, \ldots, \nu_{d+1}\}$ be a longest path in the tree $\mathbb{T}$, and let $\Delta(\mathbb{T}) \geq 3$. Moreover, suppose that $\xi_{\mathbb{T}}(\nu_2) \geq 2$.

Case 2.1: Suppose that $\xi_{\mathbb{T}}(\nu_2) = \eta$, where $\eta \in \{2, 3\}$, and let the neighborhood of ν_2 be given by $N(\nu_2) = \{\nu_1, \nu_3, \nu\}$. Consider $\mathbb{T}' = \mathbb{T} \setminus \{\nu_1\}$. In this case, the MetDim of the tree remains invariant, that is, $\dim(\mathbb{T}') = \dim(\mathbb{T})$. As a result, we obtain:

$$\begin{aligned} H_1(\mathbb{T}) &= H_1(\mathbb{T}') + 2\eta, \\ &\geq 4(\mathtt{n}-1) + \dim(\mathbb{T}) - 7 + 2\eta, \\ &= \mathbb{f}_{lb}(\mathtt{n},\ \dim(\mathbb{T})) + 2\eta - 4, \\ &\geq \mathbb{f}_{lb}(\mathtt{n},\ \dim(\mathbb{T})). \end{aligned}$$

Case 2.2: Let $\xi_{\mathbb{T}}(\nu_2) = \nu \geq 4$, and suppose the neighborhood of ν_2 is $N(\nu_2) = \{\nu_1, \nu_3, \nu_1, \ldots, \nu_{v-2}\}$. Define $\mathbb{T}' = \mathbb{T} \setminus \{\nu_1\}$. In this situation, the parameter dim decreases by exactly one, that is, $\dim(\mathbb{T}') = \dim(\mathbb{T}) - 1$. Correspondingly, we obtain:

$$\begin{aligned} H_1(\mathbb{T}) =& H_1(\mathbb{T}') + 2\nu, \\ \geq& 4(\mathtt{n}-1) + \dim(\mathbb{T}) - 8 + 2\nu, \\ =& \mathbb{f}_{lb}(\mathtt{n},\ \dim(\mathbb{T})) + 2\nu - 5, \\ >& \mathbb{f}_{lb}(\mathtt{n},\ \dim(\mathbb{T})). \end{aligned}$$

We have now completed the proof. □

Theorem 4.2. Suppose that $\mathbb{T}$ is a tree of order $\mathtt{n}$, and MetDim $\dim(\mathbb{T})$. Then, first Zagreb index $H_1(\mathbb{T})$ of $\mathbb{T}$ has following inequality:

$$H_1(\mathbb{T}) \leq (\mathtt{n}-2)(\mathtt{n}-1) + \dim(\mathbb{T}) + \mathtt{n}.$$

Proof. Suppose that $\mathbb{f}_{ub}(\mathtt{n},\ \dim(\mathbb{T})) = H_1(\mathbb{T}) \leq (\mathtt{n}-2)(\mathtt{n}-1) + \dim(\mathbb{T}) + \mathtt{n}$. This will be demonstrated by an inductive method of order n. When n resulting in a set that has cardinality of at least 4, using Theorems 2.2 and 2.4, we have that $H_1(\mathbb{P}_4) = 11 < \mathbb{f}_{lb}(4, 1)$. Meanwhile, when n offers a set with the cardinality of at least 4, then also, $H_1(\mathbb{S}_4) = 12 = \mathbb{f}_{lb}(4, 2)$. In that case, the result is valid for every $\mathbb{T}$ of order $\mathtt{n} - 1$. Suppose that we want to prove it true of a $\mathbb{T}$ with order $\mathtt{n}$. Thus, we prove here, in the following two cases, Theorem 4.2:

Case 1: Suppose we are in a position that $\Delta(\mathbb{T}) = \mathtt{n} - 1$, then we can have $\mathbb{T} \cong \nu_{\mathtt{n}}$. We may compute $H_1(\nu_{\mathtt{n}})$ using Theorem 2.2 and we also compute $\dim(\nu_{\mathtt{n}})$ using Theorem 2.4.

$$\begin{aligned} H_1(\nu_{\mathtt{n}}) &= \mathtt{n}(\mathtt{n}-1), \\ &= \mathtt{n}(\mathtt{n}-1) - (\mathtt{n}-2) + \dim(\mathbb{S}_{\mathtt{n}}), \\ &= \mathtt{n}^2 - 2\mathtt{n} + 2 + \dim(\mathbb{S}_{\mathtt{n}}), \\ &= (\mathtt{n}-1)(\mathtt{n}-2) + \dim(\mathbb{S}_{\mathtt{n}}) + \mathtt{n}, \\ &= \mathbb{f}_{ub}(\mathtt{n}, \dim(\mathbb{S}_{\mathtt{n}})). \end{aligned}$$

By having $\mathbb{T} \cong \mathbb{S}_{\mathtt{n}}$ ensures that equality is attained. Thus, whenever $T \cong \mathbb{S}_{\mathtt{n}}$, $H_1(\mathbb{T})$ attains its maximal value.

Case 2: Consider the path $\mathbb{P}_{d+1} = \{\nu_1, \nu_2, \ldots, \nu_{d+1}\}$, which realizes the diameter of the tree $\mathbb{T}$, and suppose that $\Delta(\mathbb{T}) \geq 3$. Additionally, let $\xi_{\mathbb{T}}(\nu_2) \geq 2$.

Case 2.1: Let $\xi_{\mathbb{T}}(\nu_2) = \eta$, where $\eta \in \{2, 3\}$, and suppose that the tree has order at least 5. The neighborhood of ν_2 is $N(\nu_2) = \{\nu_1, \nu_3, \nu\}$. Consider $\mathbb{T}' = \mathbb{T} \setminus \{\nu_1\}$. In this case, the parameter dim remains invariant, i.e., $\dim(\mathbb{T}') = \dim(\mathbb{T})$. Accordingly, we arrive at the following conclusion:

$$\begin{aligned} H_1(\mathbb{T}) &= H_1(\mathbb{T}') + 2\eta, \\ &\leq (\mathtt{n}-2)(\mathtt{n}-3) + \dim(\mathbb{T}) + \mathtt{n} + 2\eta - 1, \\ &= \mathbb{f}_{ub}(\mathtt{n},\ \dim(\mathbb{T})) - 2\mathtt{n} + 2\eta + 3, \\ &< \mathbb{f}_{ub}(\mathtt{n},\ \dim(\mathbb{T})). \end{aligned}$$

Case 2.2: Assume that $\xi_{\mathbb{T}}(\nu_2) = \nu \geq 4$, and let ν_2 be adjacent to the vertices $N(\nu_2) = \{\nu_1, \nu_3, \nu_1, \ldots, \nu_{\nu-2}\}$. If we construct a new tree $\mathbb{T}'$ by removing the vertex ν_1 from $\mathbb{T}$, that is, $\mathbb{T}' = \mathbb{T} \setminus \{\nu_1\}$, then the value of $\dim(\mathbb{T})$ decreases by one, resulting in $\dim(\mathbb{T}') = \dim(\mathbb{T}) - 1$. This implies that:

$$\begin{aligned} H_1(\mathbb{T}) &= H_1(\mathbb{T}') + 2\nu, \\ &\leq \mathtt{n}^2 - 2\mathtt{n} + 2 + \dim(\mathbb{T}) - 2\mathtt{n} + 2\nu + 2, \\ &= \mathbb{f}_{ub}(\mathtt{n},\ \dim(\mathbb{T})) - 2\mathtt{n} + 2\nu + 2, \\ &< \mathbb{f}_{ub}(\mathtt{n},\ \dim(\mathbb{T})). \end{aligned}$$

We have now completed the proof. □

Theorem 4.3. Let $\mathbb{T}$ be any tree of order $\mathtt{n}$ and with the MetDim $\dim(\mathbb{T})$. The second inequality is $H_2(\mathbb{T}) \geq 4\mathtt{n} + \dim(\mathbb{T}) - 9$.

Proof. Let $\mathbb{f}_{lb}(\mathtt{n},\ \dim(\mathbb{T})) = 4\mathtt{n} - 9 + \dim(\mathbb{T})$ be a function. The result will be proven by means of induction on the order of $\mathtt{n}$. Using 2.1 and 2.3 in the base case, i.e., n has a lower bound of 4, implies that $H_2(\mathbb{P}_4) = 8 = \mathbb{f}_{lb}(4, 1)$. In a similar manner, by utilizing Theorems 2.2 and 2.4, we obtain that $H_1(\mathbb{S}_4) = 9 \geq \mathbb{f}_{lb}(4, 2)$.

Suppose that the assertion holds for all trees of order $\mathtt{n} - 1$, and with this hypothesis, we shall prove the assertion of a tree of order $\mathtt{n}$. The proof will consist of the following scenarios:

Case 1: Suppose that $\Delta(\mathbb{T}) = 2$, or equivalent, $\mathbb{T} \cong \mathbb{P}_{\mathtt{n}}$. Using Theorem 2.1, we compute $H_1(\mathbb{P}_{\mathtt{n}})$, and using Theorem 2.3 we compute $\dim(\mathbb{P}_{\mathtt{n}})$:

$$\begin{aligned} H_2(\mathbb{P}_{\mathtt{n}}) &= 4\mathtt{n} - 8, \\ &= 4\mathtt{n} - 8 + \dim(\mathbb{P}_{\mathtt{n}}) - 1, \\ &= 4\mathtt{n} - 9 + \dim(\mathbb{P}_{\mathtt{n}}), \\ &= \mathbb{f}_{lb}(\mathtt{n},\ \dim(\mathbb{T})). \end{aligned}$$

Hence, the minimum value of $H_2(\mathbb{T})$ is attained precisely when $\mathbb{T}$ is isomorphic to the path $\mathbb{P}_{\mathtt{n}}$. It follows that $H_2(\mathbb{T})$ achieves its lowest value when $\mathbb{T} \cong \mathbb{P}_{\mathtt{n}}$.

Case 2: Let $\mathbb{P}_{d+1} = \{\nu_1, \nu_2, \ldots, \nu_{d+1}\}$ denote a longest path in the tree $\mathbb{T}$. We assume that the tree has maximum degree $\Delta(\mathbb{T}) \geq 3$, with the additional condition that the degree of ν_2 satisfies $\xi_{\mathbb{T}}(\nu_2) \geq 2$.

Case 2.1: Considering that the neighborhood of ν_2 equal to $N(\nu_2) = \{\nu_1, \nu_3, \nu\}$, suppose that $\xi_{\mathbb{T}}(\nu_2) = \eta$ and $\eta \in \{2, 3\}$. When $\mathbb{T}' = \mathbb{T} - \{\nu_1\}$ the MetDim is the same, i.e., $\dim(\mathbb{T}') = \dim(\mathbb{T})$. As a result, we obtain:

$$\begin{aligned} H_2(\mathbb{T}) &= H_2(\mathbb{T}') + 2\eta, \\ &\geq 4(\mathtt{n}-1) - 9 + \dim(\mathbb{T}) + 2\eta, \\ &= \mathbb{f}_{lb}(\mathtt{n},\ \dim(\mathbb{T})) + 2\eta - 4, \\ &\geq \mathbb{f}_{lb}(\mathtt{n},\ \dim(\mathbb{T})). \end{aligned}$$

Case 2.2: Continuing in this vein, suppose that we shall have $\xi_{\mathbb{T}}(\nu_2) = \nu$ so that $\nu \geq 4, N(\nu_2) = \{\nu_1, \nu_3, \nu_1, \ldots, \nu_{\nu-2}\}$. Here, in case we consider that $\mathbb{T}' = \mathbb{T} \setminus \{\nu_1\}$, then the MetDim reduces, yielding $\dim(\mathbb{T}') = \dim(\mathbb{T}) - 1$. We may then present:

$$\begin{aligned} H_2(\mathbb{T}) &= H_2(\mathbb{T}') + 2\nu, \\ &\geq 4(\mathtt{n}-1) - 9 + \dim(\mathbb{T}) - 1 + 2\nu, \\ &= \mathbb{f}_{lb}(\mathtt{n},\ \dim(\mathbb{T})) + 2\nu - 5, \\ &> \mathbb{f}_{lb}(\mathtt{n},\ \dim(\mathbb{T})). \end{aligned}$$

As a result, the statement is confirmed. □

Theorem 4.4. Suppose that $\mathbb{T}$ be a tree with order $\mathtt{n}$ and MetDim $\dim(\mathbb{T})$. Then,

$$H_2(\mathbb{T}) \leq \mathtt{n}^2 - 3\mathtt{n} + \dim(\mathbb{T}) + 3.$$

Proof. Let the upper bound function is given by $\mathbb{f}_{ub}(\mathtt{n},\ \dim(\mathbb{T})) = \mathtt{n}^2 - 3\mathtt{n} + \dim(\mathbb{T}) + 3$. We aim to prove this expression using mathematical induction on the order $\mathtt{n}$ of the tree. For the initial step $\mathtt{n} = 4$, utilizing Theorems 2.2 and 2.4, we observe that $H_2(\mathbb{P}_4) = 8 < \mathbb{f}_{ub}(4, 1)$ and $H_2(\mathbb{S}_4) = 9 = \mathbb{f}_{ub}(4, 2)$.

Suppose now that the claim holds for any tree $\mathbb{T}$ of order $\mathtt{n} - 1$, then we shall now prove it for one having the order n. Theorem 4.4 will be demonstrated in the following two:

Case 1: Assume that the maximum degree of the tree satisfies $\Delta(\mathbb{T}) = \mathtt{n} - 1$, therefore $\mathbb{T} \cong \mathbb{S}_{\mathtt{n}}$. By applying Theorem 2.2, we compute the value of $H_2(\mathbb{S}_{\mathtt{n}})$, and using Theorem 2.4, we obtain the corresponding value of $\dim(\mathbb{S}_{\mathtt{n}})$:

$$\begin{aligned} H_2(\mathbb{S}_{\mathtt{n}}) &= (\mathtt{n}-1)^2, \\ &= (\mathtt{n}-1)^2 + \dim(\mathbb{S}_{\mathtt{n}}) - (\mathtt{n}-2), \\ &= \mathtt{n}^2 - 2\mathtt{n} + 1 + \dim(\mathbb{S}_{\mathtt{n}}) - \mathtt{n} + 2, \\ &= \mathtt{n}^2 - 3\mathtt{n} + \dim(\mathbb{S}_{\mathtt{n}}) + 3, \\ &= \mathbb{f}_{ub}(\mathtt{n}, \dim(\mathbb{S}_{\mathtt{n}})). \end{aligned}$$

Notably, equality occurs if and only if $\mathbb{T} \cong \mathbb{S}_{\mathtt{n}}$. Thus, we conclude that if $\mathbb{T} \cong \mathbb{S}_{\mathtt{n}}$, then $H_2(\mathbb{T})$ is maximized.

Case 2: Let $\mathbb{P}_{d+1} = \{\nu_1, \nu_2, \ldots, \nu_{d+1}\}$ a longest path in the tree $\mathbb{T}$. Let $\Delta(\mathbb{T}) \geq 3$, with the additional condition that the degree of ν_2 satisfies $\xi_{\mathbb{T}}(\nu_2) \geq 2$.

Case 2.1: Put $\xi_{\mathbb{T}}(\nu_2) = \eta$, with $\eta = 2, 3$, and consider the order of tree at least 5 and $N(\nu_2) = \{\nu_1, \nu_3, \nu\}$. Let $\mathbb{T}' = \mathbb{T} \setminus \{\nu_1\}$, we observe similarly that the value of $\dim(\mathbb{T})$ would not change, i.e., that $\dim(\mathbb{T}') = \dim(\mathbb{T})$. We may, therefore, establish:

$$\begin{aligned} H_2(\mathbb{T}) &= H_2(\mathbb{T}') + 2\eta, \\ &\leq (\mathtt{n}-1)^2 - 3(\mathtt{n}-1) + \dim(\mathbb{T}) + 3 + 2\eta, \\ &= \mathbb{f}_{ub}(\mathtt{n},\ \dim(\mathbb{T})) - 2\mathtt{n} + 2\eta + 4, \\ &\leq \mathbb{f}_{ub}(\mathtt{n},\ \dim(\mathbb{T})). \end{aligned}$$

Case 2.2: Consider the vertex where $\xi_{\mathbb{T}}(\nu_2) = \nu \geq 4$, and the set of vertices adjacent to ν_2 is $N(\nu_2) = \{\nu_1, \nu_3, \nu_1, \ldots, \nu_{v-2}\}$. Let $\mathbb{T}'$ be the tree obtained by deleting vertex ν_1 from $\mathbb{T}$, that is, $\mathbb{T}' = \mathbb{T} \setminus \{\nu_1\}$. This deletion results in a decrease of the parameter $\dim(\mathbb{T})$ by one. Consequently, we arrive at the relation: $\dim(\mathbb{T}') = \dim(\mathbb{T}) - 1$.

$$\begin{aligned} H_2(\mathbb{T}) &= H_2(\mathbb{T}') + 2\nu, \\ &\leq \mathtt{n}^2 - 3\mathtt{n} + 3 + \dim(\mathbb{T}) - 2\mathtt{n} + 3 + 2\nu, \\ &= \mathbb{f}_{ub}(\mathtt{n},\ \dim(\mathbb{T})) - 2\mathtt{n} + 2\nu + 3, \\ &< \mathbb{f}_{ub}(\mathtt{n},\ \dim(\mathbb{T})). \end{aligned}$$

We have now completed the proof. $\square$

5 Conclusion

In this work, we investigated the influence of the MetDim on three fundamental degree-based topological indices: the first Zagreb index, the second Zagreb index, and the ABC index, within the class of tree graphs. Sharp upper and lower bounds for the Zagreb indices, as well as an upper bound for the ABC index, were established in terms of the order and MetDim of trees. Notably, our results reveal that path graphs attain the minimum values of the Zagreb indices. In contrast, star graphs maximize both the Zagreb indices and the ABC index, thereby serving as extremal structures with respect to these measures.

These results provide valuable insights into the interplay between structural parameters and degree-based indices, highlighting the significant role of the MetDim in shaping extremal behavior in trees. From an applied perspective, the derived bounds are particularly relevant to chemical graph theory, where such indices function as molecular descriptors in QSPR and QSAR studies. Furthermore, this work enriches the theoretical understanding of topological indices. It also opens avenues for future research on broader graph families and the impact of additional structural invariants on degree-based descriptors.

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References

[1] A. Ali, K. C. Das, D. Dimitrov & B. Furtula (2021). Atom-bond connectivity index of graphs: a review over extremal results and bounds. *Discrete Mathematics Letters*, *5*(1), 68–93. https://doi.org/10.47443/dml.2020.0069.

[2] W. Ali, M. N. Husin & M. F. Nadeem (2025). Extremal bounds of the atom-bond connectivity index in trees with a fixed roman domination number. *Malaysian Journal of Mathematical Sciences*, *19*(4), 1197–1210. https://doi.org/10.47836/mjms.19.4.01.

[3] W. Ali, M. N. Husin, M. F. Nadeem & M. Jabin (2025). Lower bound for the second Hyper-Zagreb index of trees with a given roman domination number. *Mathematics and Statistics*, *13*(*1*), 12–16. https://doi.org/10.13189/ms.2025.130102.

[4] A. R. Ashrafi, T. Dehghan-Zadeh & N. Habibi (2015). Extremal atom-bond connectivity index of cactus graphs. *Communications of the Korean Mathematical Society*, *30*(3), 283–295.

[5] B. Borovicanin (2015). 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*, *74*(1), 57–79.

[6] B. Borovićanin & B. Furtula (2016). On extremal Zagreb indices of trees with given domination number. *Applied Mathematics and Computation*, *279*, 208–218. https://doi.org/10.1016/j.amc.2016.01.017.

[7] G. Chartrand, L. Eroh, M. A. Johnson & O. R. Oellermann (2000). Resolvability in graphs and the metric dimension of a graph. *Discrete Applied Mathematics*, *105*(1-3), 99–113. https://doi.org/10.1016/S0166-218X(00)00198-0.

[8] J. Chen & X. Guo (2011). Extreme atom-bond connectivity index of graphs. *MATCH Communications in Mathematical and in Computer Chemistry*, *65*(3), 713–722.

[9] X. Chen & K. C. Das (2018). Solution to a conjecture on the maximum abc index of graphs with given chromatic number. *Discrete Applied Mathematics*, *251*, 126–134. https://doi.org/10.1016/j.dam.2018.05.063.

[10] K. C. Das, J. M. Rodríguez & J. M. Sigarreta (2020). On the maximal general ABC index of graphs with given maximum degree. *Applied Mathematics and Computation*, *386*, Article ID: 125531. https://doi.org/10.1016/j.amc.2020.125531.

[11] N. Dehgardi & T. Došlić (2024). Lower bounds on the general first Zagreb index of graphs with low cyclomatic number. *Discrete Applied Mathematics*, *345*, 52–61. https://doi.org/10.1016/j.dam.2023.11.033.

[12] M. Enteshari & B. Taeri (2021). Extremal Zagreb indices of graphs of order n with p pendent vertices. *MATCH Communications in Mathematical and in Computer Chemistry*, *86*, 17–28.

[13] E. Estrada, L. Torres, L. Rodriguez & I. Gutman (1998). An atom-bond connectivity index: modelling the enthalpy of formation of alkanes. *Indian Journal of Chmistry*, *33A*, 849–855.

[14] B. Furtula, A. Graovac & D. Vukičević (2009). Atom–bond connectivity index of trees. *Discrete Applied Mathematics*, *157*(13), 2828–2835. https://doi.org/10.1016/j.dam.2009.03.004.

[15] I. Gutman & K. C. Das (2004). The first Zagreb index 30 years after. *MATCH Communications in Mathematical and in Computer Chemistry*, *50*(1), 83–92. https://typeset.io/papers/the-zagreb-indices-30-years-after-22kmz1ftka.

[16] I. Gutman & N. Trinajstić (1972). Graph theory and molecular orbitals. total φ-electron energy of alternant hydrocarbons. *Chemical physics letters*, *17*(4), 535–538. https://doi.org/10.1016/0009-2614(72)85099-1.

[17] F. Harary & R. A. Melter (1976). On the metric dimension of a graph. *ArsCombinatoria*, *2*(1), 191–195.

[18] S. Ji & S. Wang (2018). On the sharp lower bounds of Zagreb indices of graphs with given number of cut vertices. *Journal of Mathematical Analysis and Applications*, *458*(1), 21–29. https://doi.org/10.1016/j.jmaa.2017.09.005.

[19] S. Li & M. Zhang (2011). Sharp upper bounds for Zagreb indices of bipartite graphs with a given diameter. *Applied mathematics letters*, *24*(2), 131–137. https://doi.org/10.1016/j.aml.2010.08.032.

[20] S. Li & H. Zhou (2010). On the maximum and minimum Zagreb indices of graphs with connectivity at most k]˙ *Applied mathematics letters*, *23*(2), 128–132. https://doi.org/10.1016/j.aml.2009.08.015.

[21] W. Lin, T. Gao, Q. Chen & X. Lin (2013). On the minimal abc index of connected graphs with given degree sequence. *MATCH Communications in Mathematical and in Computer Chemistry*, *69*(3), 571–578.

[22] D. A. Mojdeh, M. Habibi, L. Badakhshian & Y. Rao (2019). Zagreb indices of trees, unicyclic and bicyclic graphs with given (total) domination. *IEEE Access*, *7*, 94143–94149. https://doi.org/10.1109/ACCESS.2019.2927288.

[23] L. Pei & X. Pan (2018). Extremal values on Zagreb indices of trees with given distance k-domination number. *Journal of Inequalities and Applications*, *2018*, 1–17. https://doi.org/10.1186/s13660-017-1597-3.

[24] P. J. Slater (1975). Leaves of trees. *Congressus Numerantium*, *14*(549-559), 37.

[25] R. Todeschini & V. Consonni. *Handbook of molecular descriptors*.

[26] T. S. Vassilev & L. J. Huntington (2012). On the minimum ABC index of chemical trees. *Applied Mathematics*, *2*(1), 8–16. https://doi:10.5923/j.am.20120201.02.

[27] D. B. West et al. (2001). *Introduction to graph theory* volume 2. Prentice hall Upper Saddle River,. https://books.google.com.my/books?id=TuvuAAAAMAAJ.

[28] X. Wu & L. Zhang (2019). On structural properties of ABC-minimal chemical trees. *Applied Mathematics and Computation*, *362*, Article ID: 124570. https://doi.org/10.1016/j.amc.2019.124570.