Extremal Values of the Atom-Bond Connectivity Index for Trees with Given Roman Domination Numbers

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Abstract

Consider that $\mathbb{G} = (\mathbb{X}, \mathbb{Y})$ is a simple, connected graph with $\mathbb{X}$ as the vertex set and $\mathbb{Y}$ as the edge set. The atom-bond connectivity (ABC) index is a novel topological index that Estrada introduced in Estrada et al. (1998). It is defined as

$$ABC(\mathbb{G}) = \sum_{xy \in Y(\mathbb{G})} \sqrt{\frac{\zeta_x + \zeta_y - 2}{\zeta_x \zeta_y}}$$

where ζ_x and ζ_x represent the degrees of the vertices x and y, respectively. In this work, we explore the behavior of the ABC index for tree graphs. We establish both lower and upper bounds for the ABC index, expressed in terms of the graph's order and its Roman domination number. Additionally, we characterize the tree structures that correspond to these extremal values, offering a deeper understanding of how the Roman domination number (RDN) influences the ABC index in tree graphs.

Key words: ABC index; Roman domination number, Tree, chemical graph theory, Extremal values.

1 Introduction

In theoretical chemistry, mathematical chemistry is the study of chemistry without reference to quantum mechanics, aimed at explaining and predicting the properties of molecules. Graph theory is used to represent chemical events in the important topic of chemical graph theory within mathematical chemistry. The chemical sciences have advanced significantly as a result of this strategy.

A molecular graph is a fundamental graph where the edges represent bonds between atoms, and the vertices represent the atoms themselves. Hydrogen atoms are often omitted from these representations. According to IUPAC terminology, a topological index is a number associated with the chemical structure. This value is used to establish correlations between different physical and chemical attributes, biological activity, and chemical reactivity, and the chemical structure, see [13, 15–17, 22].

The Randić connectivity index is one of the most well-known topological indices, supported by a solid mathematical foundation and widely applied in pharmacology and chemistry. In 1998, Estrada et al. [11] introduced the $ABC(\mathbb{G})$ index as a notable alternative to the Randić index. According to Furtula [12], the ABC index ranks among the leading degree-based molecular descriptors.

$$ABC(\mathbb{G}) = \sum_{xy \in Y(\mathbb{G})} \sqrt{\frac{\zeta_x + \zeta_y - 2}{\zeta_x \zeta_y}} \tag{1}$$

where $Y(\mathbb{G})$ represents the set of edges in the graph $\mathbb{G}$, and ζ_x and ζ_y are the degrees of the vertices x and y connected by the edge xy. The index has been widely used to predict molecular stability, boiling points, and other properties, and has proven to be a valuable tool in QSAR/QSPR studies and drug design. Chen and

Das [7] confirmed the conjecture that the Turán graph maximizes the ABC index among graphs with a given chromatic number, resolving a problem posed by Zhang et al. [28]. Zheng et al. [30] established bounds for the general ABC index for connected graphs with fixed maximum degree, characterizing the extremal graphs for specific parameter ranges. Numerous studies have been conducted on this topological indicator, and research on it is still ongoing, see [5, 6, 19, 20, 23].

Prior research [9, 10, 27] has investigated the relations between different topological indices and the ABC index. Among other notable studies, Das and Trinajstić [10] looked at the relationship between the GA and ABC index. Xinli Xu [27] established correlations between the Harmonic index and several other indices, including the ABC index, Randić index, and the first Zagreb index, based on the order, size, and number of pendant vertices in the graph. Further research was done on the connection between the ABC index and the distance-based variation of the $ABC_{\mathbb{G}}$ index by Das et al. [9]. Additionally, they determined which extremal trees reach these limits. In order to determine the structures of extremal graphs, Zhang et al. [29] investigated the extremal limits of the ABS index for trees with certain matching and dominance values. In order to find graphs with the highest and least values of these indices, Wang et al. [24] looked into extremal multiplicative Zagreb indices in graphs with provided vertices and cut edges. Jamri et al. [2, 14] established both the extreme values of the $RI(\mathbb{T})$ with a specified TDN. Most recently, Bermudo et al. [3, 4] provided an maximum value for the $GA(\mathbb{T})$, based on their order and TDN, as well as both extreme values for the $RI(\mathbb{T})$, based on their order and domination number, and research on the bounds of various topological indices with given parameters is still ongoing, as noted in [1, 18, 21, 25].

In this study, we take a look at a simple, uncorrected connected graph $\mathbb{G}$, which has a set of vertices $\mathbb{X}$ and an edge set $\mathbb{Y}$. An edge in graph $\mathbb{G}$ connecting two vertices, x and y, is represented by the symbol xy. The open neighborhood of any vertex $y \in \mathbb{X}$ is defined as $N(y) = x \in \mathbb{X} \mid xy \in \mathbb{Y}$, whereas $N[y] = N(y) \cup y$ indicates the closed neighbor. The size of an open neighborhood, $|N(x)|$, around a vertex x, denoted by ζ_x, is called its degree. A vertex x is called a leaf if $\zeta_x = 1$. The longest path between any two leaves in a tree is defined as its diameter. A diameter path in a tree $\mathbb{T}$ is denoted by $P_{d+1} = x_1, x_2, \ldots, x_{d+1}$, where the path between vertices $x_1, x_2, \ldots, x_{d+1}$ reaches this maximum length.

For a given vertex $y \in \mathbb{X}$, the graph $\mathbb{G} - y$ is obtained by removing y, which results in a new vertex set $\mathbb{X} - y$ and an edge set $\mathbb{Y} - yx \mid x \in N(y)$. Similarly, for an edge $e \in \mathbb{Y}$, the graph $\mathbb{G} - e$ retains the original vertex set $\mathbb{X}$ but removes the edge e, resulting in the edge set $\mathbb{Y} - e$.

For l vertices $x_1, \ldots, x_l$ or edges $e_1, \ldots, e_l$, we define the graph $\mathbb{G} - x_1, \ldots, x_l$ as $(\mathbb{G} - x_1, \ldots, x_{l-1}) - x_l$, and similarly, $\mathbb{G} - e_1, \ldots, e_l$ as $(\mathbb{G} - e_1, \ldots, e_{l-1}) - e_l$. The path graph $\mathbb{P}_n$, and the star graph $\mathbb{S}_n$. We direct the reader to [26] for definitions of any other notation and terminology not covered here.

The RDN of a graph $\mathbb{G}$ is the minimum weight of a Roman dominating function on $\mathbb{G}$. An RDN is a function $\aleph : \mathbb{X}(\mathbb{G}) \to 0, 1, 2$ such that every vertex $y \in \mathbb{X}(\mathbb{G})$ with $\aleph(y) = 0$ is adjacent to at least one vertex $x \in \mathbb{X}(\mathbb{G})$ where $\aleph(x) = 2$. The weight of $\aleph$ is the sum $\aleph(\mathbb{X}) = \sum_{y \in \mathbb{X}(\mathbb{G})} \aleph(y)$ [8]. Essentially, the RDN ensures that any unguarded vertex (with $\aleph(y) = 0$) is adjacent to a heavily guarded vertex (with $\aleph(x) = 2$), and it is denoted by Γ_R.

2 Preliminary Results

We introduce a number of lemmas in this section that will be utilized to demonstrate the primary theorem. Using the Mathematics program, all single and double variables function-related inequalities in these lemmas and the main theorem's proof have been confirmed.

Lemma 2.1. *Suppose* $m(a) = (a-1)\sqrt{\frac{a-1}{a}} - (a-2)\sqrt{\frac{a-2}{a-1}}$ *with* $a \geq 3$. *Then,* $m(a)$ *is increasing function.*

Proof. Suppose that $f(a) = (a-1)\sqrt{\frac{a-1}{a}}$. The derivative is $f'(a) = \sqrt{\frac{a-1}{a}} + \frac{a-1}{2a^2}\sqrt{\frac{a}{a-1}}$. The expression for $f'(a)$ is positive for $a \geq 2$. Since $f'(a) > 0$ in this range, the function is increasing. Thus, $f(a)$ is increasing for $a \geq 2$. Therefore, $m(a) = f(a) - f(a-1) \geq 0$. □

Lemma 2.2. *Suppose* $q(a) = \sqrt{\frac{a+b-2}{ab}} - \sqrt{\frac{a+b-3}{(a-1)b}}$ *with* b, *and* $a \geq 3$. *Then,* $q(a)$ *is decreasing function for any* $b \geq 2$.

Proof. We have that $q'(a) = \frac{-b+2}{2\sqrt{b}a^{\frac{3}{2}}\sqrt{a+b-2}} - \frac{-b+2}{2\sqrt{b}(a-1)^{\frac{3}{2}}\sqrt{a+b-3}} \geq 0 \iff \frac{1}{a^{\frac{3}{2}}\sqrt{a+b-2}} \geq \frac{1}{(a-1)^{\frac{3}{2}}\sqrt{a+b-3}}$. If we denote $k(b) = \frac{1}{a^{\frac{3}{2}}\sqrt{a+b-2}}$, since $k'(b) = \frac{-1}{2a^{\frac{3}{2}}(a+b-2)^{\frac{3}{2}}} < 0$ for $b \geq 2$, $k(b)$ is a decreasing function. Thus, it follows that $\frac{1}{a^{\frac{3}{2}}\sqrt{a+b-2}} < \frac{1}{(a-1)^{\frac{3}{2}}\sqrt{a+b-3}}$. Hence, we conclude that $q(a)$ is a decreasing function for $a \geq 3$ and $b \geq 2$. □

Lemma 2.3. *Suppose* $\Xi(a,b) = (a-1)\sqrt{\frac{a-1}{a}} + \sqrt{\frac{a+b-2}{ab}} - (a-2)\sqrt{\frac{a-2}{a-1}} - \sqrt{\frac{a+b-3}{(a-1)b}} > \frac{\sqrt{5}}{2\sqrt{2}}$ *with* $a \geq 3$*, and* $b \geq 2$*.*

Proof. We begin by decomposing the function $\Xi(a,b)$ into two parts, $f_1(a) = (a-1)\sqrt{\frac{a-1}{a}} - (a-2)\sqrt{\frac{a-2}{a-1}}$ and $f_2(a,b) = \sqrt{\frac{a+b-2}{ab}} - \sqrt{\frac{a+b-3}{(a-1)b}}$. By Lemma 2.1 $f_1(a)$ is increasing function and it satisfies $f_1(a) \geq 0.9258$ ($f_1(3) = 0.9258$). By Lemma 2.2 $f_2(a,b)$ is deceasing function and it satisfies $f_2(a,b) \geq -0.1296$. Since $\Xi(a,b) = f_1(a,b) + f_2(a,b)$ we conclude $\Xi(a,b) \geq 0.7962 > \frac{\sqrt{5}}{2\sqrt{2}}$. Thus, it follows that $\Xi(a,b) > \frac{\sqrt{5}}{2\sqrt{2}}$. This completes the proof. □

Lemma 2.4. *Suppose that* $p(a) = \sqrt{a-b}\sqrt{a-b-1} - \sqrt{a-b+1}\sqrt{a-b}$ *with* $a \geq 3$ *and* $b \leq \lceil \frac{2a}{3} \rceil$ *is a increasing and negative function, and* $-\sqrt{2} \leq p(a) < -1$*.*

Proof. Suppose that $k(a) = \sqrt{a-b}\sqrt{a-b-1}$ and $k'(a) = \frac{2a-2b-1}{2\sqrt{a-b-1}\sqrt{a-b}}$, so $k(a)$ is a increasing function for $a \geq 3$ and $b \leq \lceil \frac{2a}{3} \rceil$. Therefor, give function $p(a) = k(a) - k(a+1)$ is a increasing and negative function. We verified that given function hold the inequalities $-\sqrt{2} \leq p(a) < -1$. □

Lemma 2.5. *Let* $m(a) = \sqrt{a-b-1}\sqrt{a-b-2} - \sqrt{a-b+1}\sqrt{a-b}$ *with* $a \geq 4$ *and* $b \leq \lceil \frac{2a}{3} \rceil$ *is a increasing and negative function, and* $-\sqrt{6} \leq m(a) < -2$*.*

Proof. Derivative of $\alpha(a) = \sqrt{a-b-1}\sqrt{a-b-2}$ is $\alpha'(a) = \frac{2a-2b-3}{2\sqrt{a-b-2}\sqrt{a-b-1}} > 0$. Therefore, $\alpha(a)$ is a increasing function for $a \geq 4$ and $b \leq \lceil \frac{2a}{3} \rceil$. Hence, give function $m(a) = \alpha(a) - \alpha(a+2)$ is a increasing and negative function. We verified that given function hold the inequalities $-\sqrt{6} \leq m(a) < -2$. □

Theorem 2.6. [8] For the path graph P_n*, RDN is* $\Gamma_R(\mathbb{P}_n) = \left\lceil \frac{2n}{3} \right\rceil$.

3 Main Results

This section presents the extremal values of the *ABC* index of trees in terms of their Roman domination number and order. We define two functions, $\mho\min(n, \Gamma_R)$ and $\mho\max(n, \Gamma_R)$, which represent the lower and upper bounds of the *ABC* index for trees, respectively, based on the order n and the *RDN* Γ_R. The proofs of these bounds are provided in Theorems 3.2 and 3.3. Additionally, Theorems 3.4 and 3.5 identify specific graphs that achieve these exact values.

$$\mho_{min}(n, \Gamma_R) = \frac{1}{\sqrt{2}}(n-1) + \left\lceil \frac{2n}{3} \right\rceil \left(\frac{3}{4} - \frac{1}{\sqrt{2}} \right) + \Gamma_R \left(\frac{1}{\sqrt{2}} - \frac{3}{4} \right).$$
$$\mho_{max}(n, \Gamma_R) = \sqrt{n - \Gamma_R + 1}\sqrt{n - \Gamma_R} - (\Gamma_R - 2)\left(\frac{1}{2} - \frac{3}{\sqrt{5}} \right).$$

The following lemma assists in establishing the minimum value of the *ABC* index in terms of the order and its *RDN*.

Lemma 3.1. *Suppose that* $\mathbb{T}$ *is a tree graph and* Γ_R *is a RDN, a vertex* $x \in V(\mathbb{T})$ *such that* $\zeta(x) = m \geq 3$*,* $N(x) = \{y_1, y_2, \ldots, y_m\}$*,* $\zeta(y_m) = j \geq 2$*,* $\zeta(y_a) = 1$ *for every* $a \in \{1, 2, 3, \ldots, m-1\}$*. If we take* $T' = T - y_1$*, we have:*

Proof. Since $\mathbb{T}' = \mathbb{T} - y_1$, we have $ABC(\mathbb{T}) = ABC(\mathbb{T}') + (m-1)\sqrt{\frac{m-1}{m}} + \sqrt{\frac{m+j-2}{mj}} - (m-2)\sqrt{\frac{m-2}{m-1}} - \sqrt{\frac{m+j-3}{(m-1)j}} \geq \frac{1}{\sqrt{2}}(n-1) - \frac{1}{\sqrt{2}} + \left\lceil \frac{2(n-1)}{3} \right\rceil \left(\frac{3}{4} - \frac{1}{\sqrt{2}}\right) + \Gamma_R\left(\frac{1}{\sqrt{2}} - \frac{3}{4}\right) + (m-1)\sqrt{\frac{m-1}{m}} + \sqrt{\frac{m+j-2}{mj}} - (m-2)\sqrt{\frac{m-2}{m-1}} - \sqrt{\frac{m+j-3}{(m-1)j}} \geq \mho_{min}(n, \Gamma_R) + (m-1)\sqrt{\frac{m-1}{m}} + \sqrt{\frac{m+j-2}{mj}} - (m-2)\sqrt{\frac{m-2}{m-1}} - \sqrt{\frac{m+j-3}{(m-1)j}} - \frac{1}{\sqrt{2}} - \left(\frac{3}{4} - \frac{1}{\sqrt{2}}\right)$. Suppose that $\alpha(m,j) = (m-1)\sqrt{\frac{m-1}{m}} + \sqrt{\frac{m+j-2}{mj}} - (m-2)\sqrt{\frac{m-2}{m-1}} - \sqrt{\frac{m+j-3}{(m-1)j}}$. Using Lemma 2.3, we say $\alpha(m,j) > \frac{\sqrt{5}}{2\sqrt{2}}$. So, $ABC(\mathbb{T}) \geq \mho_{max}(n, \Gamma_R) + \frac{\sqrt{5}}{2\sqrt{2}} - \frac{1}{\sqrt{2}} - \left(\frac{3}{4} - \frac{1}{\sqrt{2}}\right) > \mho_{max}(n, \Gamma_R)$. □

Theorem 3.2. *Suppose that $\mathbb{T}$ be a tree graph and let Γ_R denote its RDN. Then the ABC index of $\mathbb{T}$ satisfies the inequality $ABC(\mathbb{T}) \geq \mho_{min}(n, \Gamma_R)$.*

Proof. Let us demonstrate the outcome using induction regarding the vertex count. T is either a star S_4 or a path P_4. As we have already observed, $ABC(P_4) = \mho_{min}(4,3)$, and $ABC(S_4) = 2.44 > \mho_{min}(4,3) = 2.1213$. We examine a $\mathbb{T}$ with order n and Γ_R. We consider that the inequality holds for every $\mathbb{T}$ with $n-1$ vertices. Now we prove that for when $\mathbb{T}$ has n vertices. We discuss some cases.

Case 1: We consider that $x - y - z$ is a path in $\mathbb{T}$. If x is a leaf, $\zeta(y) = m \geq 3$ and $\zeta(z) = j \geq 2$, then we apply Lemma 3.1 and get the result.

Case 2: Let $P_{d+1} = \{x_1, x_2, \ldots, x_{d+1}\}$ is a diametral path of the tree graph. Now, Let degree of x_2 is 2.

Case 2.1: Suppose that $d(x_3) = m \geq 4$, $N(x_3) = \{x_2, x_4, w_1, \ldots, w_{m-2}\}$, $d(w_\alpha) = b_\alpha \leq 2$, $\alpha = 2, \ldots, m-2$, $d(w_1) = 1$ and $d(x_4) = k$ where $3 \leq k \leq m$. If $\mathbb{T} = \mathbb{T}_1 - \{x_1, x_2, w_1\}$, then $\Gamma_R(\mathbb{T}) = \Gamma_R(\mathbb{T}_1) + 1$, we get: $ABC(\mathbb{T}) = ABC(\mathbb{T}_1) + \sum_{\alpha=1}^{m-3}\left(\frac{1}{\sqrt{b_\alpha}}\right)\left(\sqrt{\frac{m+b_\alpha-2}{m}} - \sqrt{\frac{m+b_\alpha-4}{m-2}}\right) + \frac{1}{\sqrt{k}}\left(\sqrt{\frac{m+k-2}{m}} - \sqrt{\frac{m+k-4}{m-2}}\right) + \sqrt{\frac{m-1}{m}} + \sqrt{2} \geq \frac{1}{\sqrt{2}}(n-1) - \frac{3}{\sqrt{2}} + \left\lceil \frac{2(n-3)}{3} \right\rceil \left(\frac{3}{4} - \frac{1}{\sqrt{2}}\right) + \Gamma_R\left(\frac{1}{\sqrt{2}} - \frac{3}{4}\right) - \left(\frac{1}{\sqrt{2}} - \frac{3}{4}\right) + \sum_{\alpha=1}^{m-3}\left(\frac{1}{\sqrt{b_\alpha}}\right)\left(\sqrt{\frac{m+b_\alpha-2}{m}} - \sqrt{\frac{m+b_\alpha-3}{m-1}}\right) + \frac{1}{\sqrt{k}}\left(\sqrt{\frac{m+k-2}{m}} - \sqrt{\frac{m+k-3}{m-1}}\right) + \sqrt{\frac{m-1}{m}} + \sqrt{2} \geq \mho_{min}(n, \Gamma_R) + \sum_{\alpha=1}^{m-3}\left(\frac{1}{\sqrt{b_\alpha}}\right)\left(\sqrt{\frac{m+b_\alpha-2}{m}} - \sqrt{\frac{m+b_\alpha-4}{m-2}}\right) + \frac{1}{\sqrt{k}}(\sqrt{\frac{m+k-2}{m}} - \sqrt{\frac{m+k-4}{m-2}}) + \sqrt{\frac{m-1}{m}} - \left(\frac{3}{4} - \frac{1}{\sqrt{2}}\right) - \frac{3}{\sqrt{2}} + \sqrt{2} \geq \mho_{min}(n, \Gamma_R) + \left(\frac{m-3}{\sqrt{3}}\right)\left(\sqrt{\frac{m+1}{m}} - \sqrt{\frac{m-1}{m-2}}\right) + \frac{1}{\sqrt{k}}\left(\sqrt{\frac{m+k-2}{m}} - \sqrt{\frac{m+k-4}{m-2}}\right) + \sqrt{\frac{m-1}{m}} - \frac{3}{4}$. Suppose that $\alpha(m,k) = \left(\frac{m-3}{\sqrt{3}}\right)\left(\sqrt{\frac{m+1}{m}} - \sqrt{\frac{m-1}{m-2}}\right) + \frac{1}{\sqrt{k}}\left(\sqrt{\frac{m+k-2}{m}} - \sqrt{\frac{m+k-4}{m-2}}\right) + \sqrt{\frac{m-1}{m}} - \frac{3}{4}$. $\alpha(m,k) > 0$ for $m \geq 4$ and $3 \leq k \leq m$. So, $ABC(\mathbb{T}) \geq \mho_{min}(n, \Gamma_R) + \alpha(m,k) > \mho_{min}(n, \Gamma_R)$.

Case 2.2: We assume $\zeta(x_3) = 3$, $N(x_3) = \{x_2, x_4, y_1\}$, y_1 is the leaf of the $\mathbb{T}$ and $\zeta(x_4) = k$.

Case 2.2.1: We suppose that $1 \leq k \leq 4$. If we take $\mathbb{T}_2 = \mathbb{T} - \{x_1, x_2\}$, then $\Gamma_R(\mathbb{T}) = \Gamma_R(\mathbb{T}_2) + 1$, we get: $ABC(\mathbb{T}) = ABC(\mathbb{T}_1) + \sqrt{\frac{k+1}{3k}} + \sqrt{\frac{2}{3}} \geq \frac{1}{\sqrt{2}}(n-1) - \frac{2}{\sqrt{2}} + \left\lceil \frac{2(n-2)}{3} \right\rceil \left(\frac{3}{4} - \frac{1}{\sqrt{2}}\right) + (\Gamma_R - 1)\left(\frac{1}{\sqrt{2}} - \frac{3}{4}\right) + \sqrt{\frac{k+1}{3k}} + \sqrt{\frac{2}{3}} \geq \mho_{min}(n, \Gamma_R) + \sqrt{\frac{k+1}{3k}} + \sqrt{\frac{2}{3}} - \sqrt{2} - \left(\frac{3}{4} - \frac{1}{\sqrt{2}}\right)$. Suppose that $\beta(k) = \sqrt{\frac{k+1}{3k}} + \sqrt{\frac{2}{3}} - \sqrt{2} - \left(\frac{3}{4} - \frac{1}{\sqrt{2}}\right)$. $\beta(k) > 0$ for $1 \leq k \leq 4$. Therefore, $ABC(\mathbb{T}) \geq \mho_{min}(n, \Gamma_R) + \beta(k) > \mho_{min}(n, \Gamma_R)$.

Case 2.2.2: We suppose that $k \geq 5$, $\zeta(x_5) = u$, $N(x_4) = \{x_3, x_5, y_1, \ldots, y_{k-2}\}$, $\zeta(y_1) = 1$ and $\zeta(y_a) = b_a \leq 5$ where $a = \{2, 3, \ldots, k-2\}$. If we take $\mathbb{T}_4 = \mathbb{T} - \{x_1, x_2, x_3, x_4, y_1\}$, then $\Gamma_R(\mathbb{T}) = \Gamma_R(\mathbb{T}_4) + 3$, we get: $ABC(\mathbb{T}) = ABC(\mathbb{T}_4) + \sum_{a=1}^{u-2}\sqrt{\frac{k+b_a-2}{kb_a}} - \sum_{a=1}^{u-3}\sqrt{\frac{k+b_a-3}{(k-1)b_a}} + \sqrt{\frac{k-1}{k}} + \sqrt{\frac{k+1}{3k}} + \sqrt{\frac{k+u-2}{ku}} - \sqrt{\frac{k+u-3}{(k-1)u}} + \frac{2}{\sqrt{2}} + \sqrt{\frac{2}{3}} \geq \frac{1}{\sqrt{2}}(n-1) - \frac{5}{\sqrt{2}} + \left\lceil \frac{2(n-5)}{3} \right\rceil \left(\frac{3}{4} - \frac{1}{\sqrt{2}}\right) + (\Gamma_R - 3)\left(\frac{1}{\sqrt{2}} - \frac{3}{4}\right) + \sum_{a=1}^{u-2}\sqrt{\frac{k+b_a-2}{kb_a}} - \sum_{a=1}^{u-3}\sqrt{\frac{k+b_a-3}{(k-1)b_a}} + \sqrt{\frac{k+u-2}{ku}} - \sqrt{\frac{k+u-3}{(k-1)u}} + \sqrt{\frac{k-1}{k}} + \sqrt{\frac{k+1}{3k}} + \frac{2}{\sqrt{2}} + \sqrt{\frac{2}{3}} \geq \mho_{min}(n, \Gamma_R) + \sum_{a=1}^{u-2}\sqrt{\frac{k+b_a-2}{kb_a}} - \sum_{a=1}^{u-3}\sqrt{\frac{k+b_a-3}{(k-1)b_a}} + \sqrt{\frac{k-1}{k}} + \sqrt{\frac{k+1}{3k}} + \sqrt{\frac{k+u-2}{ku}} - \sqrt{\frac{k+u-3}{(k-1)u}} + \frac{2}{\sqrt{2}} + \sqrt{\frac{2}{3}} - \frac{5}{\sqrt{2}} \geq \mho_{min}(n, \Gamma_R) + (k-2)\sqrt{\frac{k+3}{5k}} - (k-3)\sqrt{\frac{k+2}{5(k-1)}} + \sqrt{\frac{k-1}{k}} + \sqrt{\frac{k+1}{3k}} + \sqrt{\frac{k+u-2}{ku}} - \sqrt{\frac{k+u-3}{(k-1)u}} + \frac{2}{\sqrt{2}} + \sqrt{\frac{2}{3}} - \frac{5}{\sqrt{2}}$

Suppose that $\alpha(k) = (k-2)\sqrt{\frac{k+3}{5k}} - (k-3)\sqrt{\frac{k+2}{5(k-1)}} + \sqrt{\frac{k-1}{k}} + \sqrt{\frac{k+1}{3k}}$. It has been verified that $\alpha(k) > 1.57$. Now, Let $\beta(k,u) = \sqrt{\frac{k+u-2}{ku}} - \sqrt{\frac{k+u-3}{(k-1)u}}$. By using Lemma 2.2, we have $\beta(k,u) > -0.013$. Therefore,

$ABC(\mathbb{T}) \geq \mho_{min}(n, \Gamma_R) + \alpha(k) + \beta(k,u) + \frac{2}{\sqrt{2}} + \sqrt{\frac{2}{3}} - \frac{5}{\sqrt{2}} > \mho_{min}(n, \Gamma_R)$.

Case 2.3: Assume that $\zeta(x_3) = 2$, $\zeta(x_4) = l \geq 2$, and $N(x_4) = \{x_3, x_5, y_1, \ldots, y_{l-2}\}$, where $\zeta(y_i) = a_i \leq 5$ for $i \in \{1, 2, \ldots, l-2\}$ and $\zeta(x_5) = t \leq l$. If we take $\mathbb{T}_5 = \mathbb{T} - \{x_1, x_2, x_3, y_1\}$, then $\Gamma_R(\mathbb{T}) = \Gamma_R(\mathbb{T}_4) + 2$, we get: $ABC(\mathbb{T}) = ABC(\mathbb{T}_5) + \sum_{i=1}^{l-3} \frac{1}{\sqrt{a_i}} \left(\sqrt{\frac{l+a_i-2}{l}} - \sqrt{\frac{l+a_i-3}{l-1}} \right) + \sqrt{\frac{l-1}{l}} + \frac{1}{\sqrt{k}} \left(\sqrt{\frac{l+k-2}{l}} - \sqrt{\frac{l+k-3}{l-1}} \right) + \frac{3}{\sqrt{2}} \geq \frac{1}{\sqrt{2}}(n-1) - \frac{4}{\sqrt{2}} + \left\lceil \frac{2(n-4)}{3} \right\rceil \left(\frac{3}{4} - \frac{1}{\sqrt{2}} \right) + (\Gamma_R - 2) \left(\frac{1}{\sqrt{2}} - \frac{3}{4} \right) + \sum_{i=1}^{l-3} \frac{1}{\sqrt{a_i}} \left(\sqrt{\frac{l+a_i-2}{l}} - \sqrt{\frac{l+a_i-3}{l-1}} \right) + \sqrt{\frac{l-1}{l}} + \frac{1}{\sqrt{k}} \left(\sqrt{\frac{l+k-2}{l}} - \sqrt{\frac{l+k-3}{l-1}} \right) + \frac{3}{\sqrt{2}} \geq \mho_{min}(n, \Gamma_R) + \sum_{i=1}^{l-3} \frac{1}{\sqrt{a_i}} \left(\sqrt{\frac{l+a_i-2}{l}} - \sqrt{\frac{l+a_i-3}{l-1}} \right) + \sqrt{\frac{l-1}{l}} + \frac{1}{\sqrt{k}} \left(\sqrt{\frac{l+k-2}{l}} - \sqrt{\frac{l+k-3}{l-1}} \right) - \frac{1}{\sqrt{2}} - \left(\frac{3}{4} - \frac{1}{\sqrt{2}} \right) > \mho_{min}(n, \Gamma_R) + \frac{l-3}{\sqrt{5}} \left(\sqrt{\frac{l+3}{l}} - \sqrt{\frac{l+2}{l-1}} \right) + \sqrt{1 - \frac{1}{l}} + \frac{1}{\sqrt{k}} \left(\sqrt{\frac{l+k-2}{l}} - \sqrt{\frac{l+k-3}{l-1}} \right) - \frac{3}{4}$.

Let $\alpha(l) = \frac{l-3}{\sqrt{5}} \left(\sqrt{\frac{l+3}{l}} - \sqrt{\frac{l+2}{l-1}} \right) + \sqrt{1 - \frac{1}{l}}$. Since $\alpha(l)$ is an increasing function for every $l \geq 3$, we define $\beta(l,k) = \frac{1}{\sqrt{k}} \left(\sqrt{\frac{l+k-2}{l}} - \sqrt{\frac{l+k-3}{l-1}} \right)$. By Lemma 2.2 $\beta(l,k)$ is a decreasing function. Therefore, the inequality holds: $ABC(\mathbb{T}) \geq \mho_{min}(n, \Gamma_R) + \alpha(l) + \beta(l,k) - \frac{3}{4} > \mho_{min}(n, \Gamma_R)$. □

Theorem 3.3. *If $\mathbb{T}$ be a tree graph and let Γ_R denote its RDN. Then the ABC index of $\mathbb{T}$ satisfies the inequality $ABC(\mathbb{T}) \leq \mho_{max}(n, \Gamma_R)$.*

Proof. Let us demonstrate the outcome using induction regarding the vertex count. $\mathbb{T}$ is either a star S_4 or a path P_4. As we have already observed, $ABC(P_4) = 2.121 < \mho_{max}(4,3)$, and $ABC(S_4) = \mho_{max}(4,3) = 2.44$. We examine a $\mathbb{T}$ with order n and RDN Γ_R. We consider that the inequality holds for every $\mathbb{T}$ with $n-1$ vertices. Now we prove that for when $\mathbb{T}$ has n vertices. We discuss some cases.
Case 1: Consider a vertex x where $\zeta(x) = m \geq 3$, $N(x) = \{y_1, y_2, \ldots, y_m\}$, $\zeta(y_m) = j \geq 2$, $\zeta(y_a) = 1$ for every $a \in \{1, 2, 3, \ldots, m-1\}$. If we take $T' = T - y_1$, then $\Gamma_R(\mathbb{T}) = \Gamma_R(\mathbb{T}')$. We have: $ABC(\mathbb{T}) = ABC(\mathbb{T}') + \frac{1}{\sqrt{m}} \left((m-1)^{\frac{3}{2}} + \sqrt{\frac{m+j-2}{j}} \right) - \frac{1}{m-1} \left((m-2)^{\frac{3}{2}} + \sqrt{\frac{m+j-3}{j}} \right) \leq \sqrt{n - \Gamma_R}\sqrt{n - \Gamma_R - 1} - (\Gamma_R - 2) \left(\frac{1}{2} - \frac{3}{\sqrt{5}} \right) + \frac{1}{\sqrt{m}} \left((m-1)^{\frac{3}{2}} + \sqrt{\frac{m+j-2}{j}} \right) - \frac{1}{\sqrt{m-1}} \left((m-2)^{\frac{3}{2}} + \sqrt{\frac{m+j-3}{j}} \right) \leq \mho_{max}(n, \Gamma_R) + \sqrt{n - \Gamma_R} \sqrt{n - \Gamma_R - 1} - \sqrt{n - \Gamma_R + 1}\sqrt{n - \Gamma_R} + \frac{1}{\sqrt{m}} \left((m-1)^{\frac{3}{2}} + \sqrt{\frac{m+j-2}{j}} \right) - \frac{1}{\sqrt{m-1}} \left((m-2)^{\frac{3}{2}} + \sqrt{\frac{m+j-3}{j}} \right)$. We assume that $\alpha(n) = \sqrt{n - \Gamma_R}\sqrt{n - \Gamma_R - 1} - \sqrt{n - \Gamma_R + 1}\sqrt{n - \Gamma_R}$ and $\beta(m,j) = \frac{1}{\sqrt{m}} \left((m-1)^{\frac{3}{2}} + \sqrt{\frac{m+j-2}{j}} \right) - \frac{1}{\sqrt{m-1}} \left((m-2)^{\frac{3}{2}} + \sqrt{\frac{m+j-3}{j}} \right)$. By using Lemma 2.4, we get $-\sqrt{2} \leq \alpha(n) < -1$ for $n \geq 3$ and $2 \leq \Gamma_R \leq \lceil \frac{2n}{3} \rceil$ and by Lemma 2.3, we get $\frac{\sqrt{5}}{2\sqrt{2}} \leq \beta(m,j) < 1$ for any $m \geq 3$ and $j \geq 2$. Therefore, $\eta(n,m,j) = \alpha(n) + \beta(m,j)$ is negative function. So, $ABC(\mathbb{T}) \leq \mho_{max}(n, \Gamma_R) + \eta(n,m,j) < \mho_{max}(n, \Gamma_R)$.

Case 2: Let $P_{d+1} = \{x_1, x_2, \ldots, x_{d+1}\}$ is a diametral path of the tree. Let $\zeta(x_2) = 2$, $\zeta(x_3) = m$, $N(x_3) = \{x_2, x_4, y_1, \ldots, y_{m-2}\}$, $\zeta(y_i) = b_i$, where $i \in \{1, 2, \ldots, m-2\}$, and $\zeta(x_4) = k$. If we take $\mathbb{T}_2 = \mathbb{T} - \{x_1, x_2\}$, then $\Gamma_R(\mathbb{T}) = \Gamma_R(\mathbb{T}_2) + 1$, we get: $ABC(\mathbb{T}) = ABC(\mathbb{T}_2) + \frac{1}{\sqrt{k}} \left(\sqrt{\frac{m+k-2}{m}} - \sqrt{\frac{m+k-3}{m-1}} \right) + \sum_{i=1}^{m-1} \frac{1}{\sqrt{b_i}} \left(\sqrt{\frac{m+b_i-2}{m}} - \sqrt{\frac{m+b_i-3}{m-1}} \right) + \sqrt{2} \leq \sqrt{n - \Gamma_R - 1}\sqrt{n - \Gamma_R - 2} - (\Gamma_R - 3) \left(\frac{1}{2} - \frac{3}{\sqrt{5}} \right) + \frac{1}{\sqrt{k}} (\sqrt{\frac{m+k-2}{m}} - \sqrt{\frac{m+k-3}{m-1}}) + \sum_{i=1}^{m-2} \frac{1}{\sqrt{b_i}} \left(\sqrt{\frac{m+b_i-2}{m}} - \sqrt{\frac{m+b_i-3}{m-1}} \right) + \sqrt{2} \leq \mho_{max}(n, \Gamma_R) + \sqrt{n - \Gamma_R - 1}\sqrt{n - \Gamma_R - 2} - \sqrt{n - \Gamma_R + 1}\sqrt{n - \Gamma_R} + \frac{1}{\sqrt{k}} \left(\sqrt{\frac{m+k-2}{m}} - \sqrt{\frac{m+k-3}{m-1}} \right) + \sum_{i=1}^{m-2} \frac{1}{\sqrt{b_i}} \left(\sqrt{\frac{m+b_i-2}{m}} - \sqrt{\frac{m+b_i-3}{m-1}} \right) + \sqrt{2} + \left(\frac{1}{2} - \frac{3}{\sqrt{5}} \right) \leq \mho_{max}(n, \Gamma_R) + \sqrt{n - \Gamma_R - 1}\sqrt{n - \Gamma_R - 2} - \sqrt{n - \Gamma_R + 1}\sqrt{n - \Gamma_R} + \frac{1}{\sqrt{k}} \left(\sqrt{\frac{m+k-2}{m}} - \sqrt{\frac{m+k-3}{m-1}} \right) + \frac{m-2}{\sqrt{5}} \left(\sqrt{\frac{m+3}{m}} - \sqrt{\frac{m+2}{m-1}} \right) + \sqrt{2} + \left(\frac{1}{2} - \frac{3}{\sqrt{5}} \right)$.

We assume that $\alpha(n) = \sqrt{n - \Gamma_R - 1}\sqrt{n - \Gamma_R - 2} - \sqrt{n - \Gamma_R + 1}\sqrt{n - \Gamma_R}$, $\beta(m,k) = \frac{1}{\sqrt{k}} \left(\sqrt{\frac{m+k-2}{m}} - \sqrt{\frac{m+k-3}{m-1}} \right)$

and $\gamma(m) = \frac{m-2}{\sqrt{5}}\left(\sqrt{\frac{m+3}{m}} - \sqrt{\frac{m+2}{m-1}}\right)$. By using Lemma 2.5, we get $-\sqrt{6} \leq \alpha(n) < -2$, by Lemma 2.2 $\beta(m,k)$ is decreasing function, and $\gamma(m)$ is negative function for any $m \geq 3$. Hence, $ABC(\mathbb{T}) \leq \mho_{max}(n, \Gamma_R) + \alpha(n) + \beta(m,k) + \gamma(m) + \sqrt{2} + \left(\frac{1}{2} - \frac{3}{\sqrt{5}}\right) < \mho_{max}(n, \Gamma_R)$.

□

Theorem 3.4. Suppose that $\mathbb{T}$ be a tree with order n and RDN Γ_R, then we have $ABC(\mathbb{T}) = \mho_{min}(n, \Gamma_R)$ if and only if $\mathbb{T} = \mathbb{P}_n$.

Proof. Using Equation 1, we know that for the path graph $\mathbb{P}_n$, the ABC index is: $ABC(\mathbb{P}_n) = \frac{1}{\sqrt{2}}(n-1)$. By Theorem 2.6, the RDN of the path graph $\mathbb{P}_n$ is, $\Gamma_R(\mathbb{P}_n) = \lceil \frac{2n}{3} \rceil$. Substituting this into the formula for $\mho_{max}(n, \Gamma_R)$, we get $\mho_{max}(n, \Gamma_R) = \frac{1}{\sqrt{2}}(n-1) + \lceil \frac{2n}{3} \rceil \left(\frac{3}{4} - \frac{1}{\sqrt{2}}\right) + \Gamma_R(\mathbb{P}_n)\left(\frac{1}{\sqrt{2}} - \frac{3}{4}\right) = \frac{1}{\sqrt{2}}(n-1) = ABC(\mathbb{P}_n)$. □

Theorem 3.5. Suppose that $\mathbb{T}$ a tree with order n and the RDN Γ_R, then we have $ABC(\mathbb{T}) = \mho_{max}(n, \Gamma_R)$ if and only if $\mathbb{T} = S_n$.

Proof. By using Equation 1, we know that for the star graph $\mathbb{S}_n$, the ABC index in the term of order of $\mathbb{S}_n$ is given by: $ABC(\mathbb{S}_n) = \sqrt{n-1}\sqrt{n-2}$ and RDN of $\mathbb{S}_n$ is 2 ($\Gamma_R(\mathbb{S}_n) = 2$). Hence, we substitute this into the formula for $\mho_{max}(n, \Gamma_R(\mathbb{S}_n))$, giving: $\mho_{max}(n, \Gamma_R(\mathbb{S}_n)) = \sqrt{n-1}\sqrt{n-2} = ABC(\mathbb{S}_n)$. This is exactly equal to the ABC index of $\mathbb{S}_n$, so we conclude that: $ABC(\mathbb{S}_n) = \mho_{max}(n, \Gamma_R(\mathbb{S}_n))$. □

4 Conclusion

In this study, we examined the ABC index of tree graphs, focusing on its dependence on the RDN and the tree's order. We established the lower and upper bounds of the ABC index, as detailed in Theorems 3.2 and 3.3, demonstrating that these bounds are determined by the tree's order and RDN. Specifically, Theorem 3.4 shows that $\mathbb{P}_n$ achieve the minimum ABC index, while Theorem 3.5 reveals that $\mathbb{S}_n$ trees attain the maximum index, illustrating the significant impact of the RDN on these extremal values. These results enhance the understanding of the relationship between tree parameters and topological indices, providing a basis for future research to explore these interactions in broader graph classes and uncover new connections between the ABC index and other graph invariants.

Declarations

Author Contribution Statement All authors contributed equally to the paper.

Declaration of competing interest The authors have no conflict of interest to disclose.

Data availability statements All the data used to find the results is included in the manuscript.

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