

On the difference between geometric-arithmetic index and atom-bond connectivity index for trees



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Abstract

Let G be a simple and connected graph with vertex set $V(G)$ and edge set $E(G)$. The geometric-arithmetic index and atom-bond connectivity index of graph G are defined as $GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$ and $ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$, respectively, where the summation extends over all edges uv of G , and d_u denotes the degree of vertex u in G . Let $(GA - ABC)(G)$ denote the difference between GA and ABC indices of G . In this note, we determine n -vertex binary trees with first three minimum $GA - ABC$ values. We also present a lower bound for $GA - ABC$ index of molecular trees with fixed number of pendant vertices.

Keywords: Atom-bond connectivity index, geometric-arithmetic index, trees.

2020 MSC: 05C35, 05C90.

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1. Introduction

Let G be a simple and connected graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(G) = \{e_1, e_2, \dots, e_m\}$, where $|V(G)| = n$ and $|E(G)| = m$. For $u \in V(G)$, d_u denotes the degree of vertex u in G . The minimum degree and maximum degree of G are denoted by δ and Δ . Let $x, y \in V(G)$, then the distance $d_G(x, y)$ between x and y is defined as the length of any shortest path in G connecting x and y . For a vertex v_i of $V(G)$, its eccentricity e_i is the largest distance between v_i and any other vertex v_k of G , i.e., $e_i = \max_{v_j \in V(G)} d_G(v_i, v_j)$. For the notations and terminologies not mentioned here, please refer to [19].

Graph theory has provided the chemists with a variety of useful tools, one of which is the topological indices [7]. Molecules and molecular compounds are often modeled by molecular graphs. Topological indices of molecular graphs are one of the oldest and the most widely used descriptors in QSPR/QSAR research [16].

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doi: [10.22436/jmcs.022.01.05](https://doi.org/10.22436/jmcs.022.01.05)

Received: 2020-04-16 Revised: 2020-04-28 Accepted: 2020-05-16

Estrada et al. [10] proposed the *atom-bond connectivity index* of graph G which is abbreviated as $ABC(G)$ and defined as

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}},$$

where the summation goes over all edges of G . The ABC index is one of many so called topological indices that are extensively used in theoretical chemistry to correlate physico-chemical properties with the molecular structures of chemical compounds. It appears that the ABC index shows a strong correlation with heat of formation of alkanes [10]. Some topological approaches were also developed based on the ABC index to explain the differences in the energy of linear and branched alkanes [9].

In the study of topological indices in general, it is often of interest to consider the extremal values of a certain index among graphs under various constraints. Along this line, the extremal values of ABC index have been extensively explored, see [2, 8, 11, 15, 20] and the references cited therein.

Another topological index of graph G , named the *geometric-arithmetic index* and abbreviated as $GA(G)$, was introduced by Vukičević and Furtula [17] in 2009. The GA index is defined as follows

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v},$$

where the summation goes over all edges of G . It is noted in that the GA index is well correlated with a variety of physico-chemical properties and the predictive power of GA index is somewhat better than the Randić index. Until now, many mathematical properties of GA index were investigated, see the survey [5], some recent papers [3, 4, 14, 21] and the references cited therein.

In line with the great interest of topological indices, some researchers are also keen on the research of the relationship or comparison between topological indices. Das and Trinajstić [6] compared the GA index and ABC index for chemical trees, molecular trees and simple graphs with some restricted conditions. Raza et al. [13] proved that GA index is greater than ABC index for line graphs of molecular graphs, for general graphs in which the difference between maximum and minimum degree is less than or equal to $(2\delta - 1)^2$ and for some families of trees. Zhong and Cui [22] obtained a relation between these two indices for simple connected graphs on $n \geq 3$ vertices with minimum degree at least s and maximum degree at most t , where $1 \leq s \leq t \leq n - 1$ and $t \geq 2$. Using this relation, they proved that if $t \leq 4s^2 - 3s + 1$, then the ABC index is always less than the GA index and this bound is best possible for $s \geq 2$. Recently, Ke [12] and Wei et al. [18] compared the expected values of the GA index and ABC index for random polyphenyl chains and spiro chains, respectively. However, the comparison between these two indices, in the case of trees and general graphs, remains an open problem.

A tree T is said to be a binary tree (chemical tree, respectively) if the maximum vertex degree in T is at most 3 (4, respectively). Very recently, Ali and Du [1] established some extremal results with respect to the difference between ABC index and Randić index (R index for short) for binary and chemical trees. Let $(GA - ABC)(G)$ be the difference between GA index and ABC index of G . In this paper, we investigate the n -vertex binary trees with minimum $GA - ABC$ values. We also obtain a lower bound for $GA - ABC$ index of molecular trees with fixed number of pendant vertices.

2. Minimum values of $GA - ABC$ index for binary trees

In this section, we characterize the trees with extremal $GA - ABC$ values among all n -vertex binary trees.

Let $x_{i,j}$ be the number of edges in the graph G connecting the vertices of degrees i and j . Then the formula for the graph invariant $GA - ABC$ can be rewritten in terms of $x_{i,j}$ as follows

$$(GA - ABC)(G) = \sum_{\delta \leq i \leq j \leq \Delta} \frac{2ij - (i + j)(\sqrt{i + j - 2})}{(\sqrt{ij})(i + j)} x_{i,j}, \quad (2.1)$$

where δ and Δ are, respectively, the minimum and maximum degrees in G .

Let n_i be the number of vertices of degree i in G . Then the following system of equations holds for any n -vertex binary tree T (see [1, 20]):

$$n_1 + n_2 + n_3 = n, \tag{2.2}$$

$$n_1 + 2n_2 + 3n_3 = 2(n - 1), \tag{2.3}$$

$$x_{1,2} + x_{1,3} = n_1, \tag{2.4}$$

$$x_{1,2} + 2x_{2,2} + x_{2,3} = 2n_2, \tag{2.5}$$

$$x_{1,3} + x_{2,3} + 2x_{3,3} = 3n_3. \tag{2.6}$$

We solve the system of (2.2), (2.3), (2.4), (2.5), (2.6) for the unknown $n_1, n_2, n_3, x_{1,3}, x_{3,3}$. The values of $x_{1,3}$ and $x_{3,3}$ are, respectively, given as below:

$$\begin{aligned} x_{1,3} &= \frac{1}{4}(2n + 4 - 5x_{1,2} - 2x_{2,2} - x_{2,3}), \\ x_{3,3} &= \frac{1}{4}(2n - 8 + x_{1,2} - 2x_{2,2} - 3x_{2,3}). \end{aligned} \tag{2.7}$$

By substituting these values of $x_{1,3}$ and $x_{3,3}$ in (2.1), one has

$$\begin{aligned} (GA - ABC)(G) &= \frac{3\sqrt{3} - 2\sqrt{6} + 2}{12}n + \frac{3\sqrt{3} - 2\sqrt{6} - 4}{6} \\ &\quad - \frac{15\sqrt{3} - 4\sqrt{2} - 10\sqrt{6} - 2}{24}x_{1,2} - \frac{3\sqrt{3} - 2\sqrt{6} + 6\sqrt{2} - 10}{12}x_{2,2} \\ &\quad - \frac{15\sqrt{3} + 60\sqrt{2} - 58\sqrt{6} + 30}{120}x_{2,3}. \end{aligned} \tag{2.8}$$

Let

$$\begin{aligned} \wedge &= \frac{15\sqrt{3} - 4\sqrt{2} - 10\sqrt{6} - 2}{24}x_{1,2} + \frac{3\sqrt{3} - 2\sqrt{6} + 6\sqrt{2} - 10}{12}x_{2,2} \\ &\quad + \frac{15\sqrt{3} + 60\sqrt{2} - 58\sqrt{6} + 30}{120}x_{2,3}. \end{aligned} \tag{2.9}$$

Then (2.8) becomes to

$$(GA - ABC)(G) = \frac{3\sqrt{3} - 2\sqrt{6} + 2}{12}n + \frac{3\sqrt{3} - 2\sqrt{6} - 4}{6} - \wedge. \tag{2.10}$$

We note that

$$\begin{aligned} \frac{15\sqrt{3} - 4\sqrt{2} - 10\sqrt{6} - 2}{24} &\approx -0.2571245652, \\ \frac{3\sqrt{3} - 2\sqrt{6} + 6\sqrt{2} - 10}{12} &\approx -0.1014621407, \\ \frac{15\sqrt{3} + 60\sqrt{2} - 58\sqrt{6} + 30}{120} &\approx -0.01030691021. \end{aligned}$$

So to minimize $(ABC - R)(G)$, it is sufficient to search binary trees for which \wedge is maximum.

Now we present our main result.

Theorem 2.1. Consider the set of all n -vertex binary trees.

(1) Suppose that n is even.

(1.1) For $n \geq 4$, the minimum GA – ABC value is

$$\frac{3\sqrt{3}-2\sqrt{6}+2}{12}n + \frac{3\sqrt{3}-2\sqrt{6}-4}{6},$$

which is uniquely obtained by those trees that contain no vertex of degree 2, that is, $n_2 = 0$.

(1.2) For $n \geq 10$, the second minimum GA – ABC value is

$$\frac{3\sqrt{3}-2\sqrt{6}+2}{12}n + \frac{24\sqrt{6}-30\sqrt{2}-25}{15},$$

which is uniquely obtained by those trees that contain exactly two vertices of degree 2, that is, $n_2 = 2$, either of which is adjacent to two vertices of degree 3, that is, $x_{1,2} = x_{2,2} = 0$ and $x_{2,3} = 4$.

(1.3) For $n \geq 16$, the third minimum GA – ABC value is

$$\frac{3\sqrt{3}-2\sqrt{6}+2}{12}n + \frac{106\sqrt{6}-15\sqrt{3}-120\sqrt{2}-80}{30},$$

which is uniquely obtained by those trees that contain exactly four vertices of degree 2, that is, $n_2 = 4$, either of which is adjacent to two vertices of degree 3, that is, $x_{1,2} = x_{2,2} = 0$ and $x_{2,3} = 8$.

(2) Suppose that n is odd.

(2.1) For $n \geq 7$, the minimum GA – ABC value is

$$\frac{3\sqrt{3}-2\sqrt{6}+2}{12}n + \frac{15\sqrt{3}+38\sqrt{6}-60\sqrt{2}-70}{60},$$

which is uniquely obtained by those trees that contain exactly one vertex of degree 2, that is, $n_2 = 1$, which is adjacent to two vertices of degree 3, that is, $x_{1,2} = 0$ and $x_{2,3} = 2$.

(2.2) For $n \geq 13$, the second minimum GA – ABC value is

$$\frac{3\sqrt{3}-2\sqrt{6}+2}{12}n + \frac{154\sqrt{6}-15\sqrt{3}-180\sqrt{2}-130}{60},$$

which is uniquely obtained by those trees that contain exactly three vertices of degree 2, that is, $n_2 = 3$, each of which is adjacent to two vertices of degree 3, that is, $x_{1,2} = x_{2,2} = 0$ and $x_{2,3} = 6$.

(2.3) For $n \geq 19$, the third minimum GA – ABC value is

$$\frac{3\sqrt{3}-2\sqrt{6}+2}{12}n + \frac{270\sqrt{6}-45\sqrt{3}-300\sqrt{2}-190}{60},$$

which is uniquely obtained by those trees that contain exactly five vertices of degree 2, that is, $n_2 = 5$, each of which is adjacent to two vertices of degree 3, that is, $x_{1,2} = x_{2,2} = 0$ and $x_{2,3} = 10$.

Proof. If $x_{1,2} \geq 1$, then by (2.9),

$$\wedge \geq \frac{15\sqrt{3}-4\sqrt{2}-10\sqrt{6}-2}{24} \approx -0.2571245652.$$

If $x_{2,2} \geq 1$, then by (2.9),

$$\begin{aligned} \wedge &\geq \frac{3\sqrt{3}-2\sqrt{6}+6\sqrt{2}-10}{12} + (2n_2-2) \cdot \frac{15\sqrt{3}+60\sqrt{2}-58\sqrt{6}+30}{120} \\ &\approx -0.1014621407 - 0.02061382043n_2 + 0.02061382043 \end{aligned}$$

$$\begin{aligned} &\approx -0.02061382043n_2 - 0.08084832027 \\ &\geq \begin{cases} -0.02061382043 \cdot 2 - 0.08084832027 \approx -0.1220759611, & \text{if } n_2 \text{ is even,} \\ -0.02061382043 \cdot 3 - 0.08084832027 \approx -0.1426897816, & \text{if } n_2 \text{ is odd.} \end{cases} \end{aligned}$$

Suppose in the following that $x_{1,2} = x_{2,2} = 0$. Then $x_{2,3} = 2n_2$ from (2.5).

Also from (2.7), we have that $n \geq \frac{3x_{2,3}+8}{2}$. From (2.2) and (2.3), we have

$$n_2 + 2n_3 = n - 2,$$

which implies that n_2 and n have the same parity.

Case 1. n is even.

In this case, note that n_2 is also even.

If $n_2 = 0$, then $x_{2,3} = 0$, $n \geq 4$ and by (2.9), we have $\wedge = 0$.

If $n_2 = 2$, then $x_{2,3} = 4$, $n \geq 10$ and by (2.9), we have

$$\wedge = 4 \cdot \frac{15\sqrt{3} + 60\sqrt{2} - 58\sqrt{6} + 30}{120} \approx -0.04122764085.$$

If $n_2 = 4$, then $x_{2,3} = 8$, $n \geq 16$ and by (2.9), we have

$$\wedge = 8 \cdot \frac{15\sqrt{3} + 60\sqrt{2} - 58\sqrt{6} + 30}{120} \approx -0.0824552817.$$

If $n_2 \geq 6$, then $x_{2,3} \geq 12$ and by (2.9), we have

$$\wedge \geq 12 \cdot \frac{15\sqrt{3} + 60\sqrt{2} - 58\sqrt{6} + 30}{120} \approx -0.1236829226.$$

The first three maximum \wedge are 0, -0.04122764085, -0.0824552817 and thus the first three minimum GA – ABC values for n is even follow from (2.10) easily.

Case 2. n is odd.

In this case, note that n_2 is also odd.

If $n_2 = 1$, then $x_{2,3} = 2$, $n \geq 7$ and by (2.9), we have

$$\wedge = 2 \cdot \frac{15\sqrt{3} + 60\sqrt{2} - 58\sqrt{6} + 30}{120} \approx -0.02061382043.$$

If $n_2 = 3$, then $x_{2,3} = 6$, $n \geq 13$ and by (2.9), we have

$$\wedge = 6 \cdot \frac{15\sqrt{3} + 60\sqrt{2} - 58\sqrt{6} + 30}{120} \approx -0.06184146128.$$

If $n_2 = 5$, then $x_{2,3} = 10$, $n \geq 19$ and by (2.9), we have

$$\wedge = 10 \cdot \frac{15\sqrt{3} + 60\sqrt{2} - 58\sqrt{6} + 30}{120} \approx -0.1030691021.$$

If $n_2 \geq 7$, then $x_{2,3} \geq 14$ and by (2.9), we have

$$\wedge \geq 14 \cdot \frac{15\sqrt{3} + 60\sqrt{2} - 58\sqrt{6} + 30}{120} \approx -0.144296743.$$

The first three maximum \wedge are -0.02061382043, -0.06184146128, -0.1030691021 and thus the first three minimum GA – ABC values for n is odd follow from (2.10) easily.

□

The binary trees in Theorem 2.1 with the smallest number of vertices are listed in Figures 1 and 2.

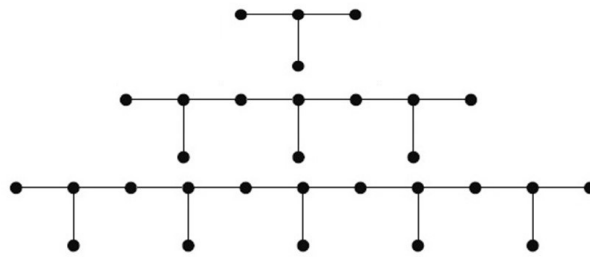


Figure 1: The binary trees in Theorem 2.1 (1.1), (1.2) and (1.3) with $n = 4, 10, 16$, respectively.

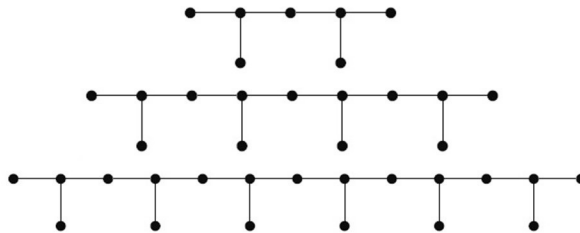


Figure 2: The binary trees in Theorem 2.1 (2.1), (2.2) and (2.3) with $n = 7, 13, 19$, respectively.

3. Upper bound for GA – ABC index of molecular trees

For a molecular tree T on n vertices, denote by n_i the number of vertices in T with degree i for $i = 1, 2, 3, 4$. The following system of equations holds for any T (see [1, 20]):

$$\begin{aligned} n_1 + n_2 + n_3 + n_4 &= n, \\ n_1 + 2n_2 + 3n_3 + 4n_4 &= 2(n - 1), \\ x_{1,2} + x_{1,3} + x_{1,4} &= n_1, \\ x_{1,2} + 2x_{2,2} + x_{2,3} + x_{2,4} &= 2n_2, \\ x_{1,3} + x_{2,3} + 2x_{3,3} + x_{3,4} &= 3n_3, \\ x_{1,4} + x_{2,4} + x_{3,4} + 2x_{4,4} &= 4n_4. \end{aligned} \tag{3.1}$$

Let \mathcal{T}_{n,n_1} be the set of molecular trees with satisfy

$$\begin{aligned} x_{1,4} &= n_1, \\ x_{2,2} &= n - 2n_1 + 3 - \frac{1}{3}x_{2,3}, \\ x_{2,4} &= n_1 - 4 - \frac{2}{3}x_{2,3}, \\ n_2 &= n - \frac{3}{2}n_1 + 1 - \frac{1}{6}x_{2,3}, \\ n_3 &= \frac{1}{3}x_{2,3}, \end{aligned}$$

and

$$n_4 = \frac{1}{2}n_1 - 1 - \frac{1}{6}x_{2,3}.$$

Theorem 3.1 ([20]). *Let T be a molecular tree with n vertices, $n_1 \geq 5$ of which are pendant vertices. Then*

$$ABC(G) \leq \frac{\sqrt{2}}{2}n + \frac{\sqrt{3}-\sqrt{2}}{2}n_1 - \frac{\sqrt{2}}{2},$$

with equality holds if and only if $T \in \mathcal{T}_{n,n_1}$.

Obviously, from (3.1) we obtain

$$\begin{aligned} (GA - ABC)(T) &= \frac{1}{3\sqrt{2}}x_{1,2} + \frac{6-4\sqrt{2}}{4\sqrt{3}}x_{1,3} + \frac{8-5\sqrt{3}}{10}x_{1,4} + \frac{8-4\sqrt{2}}{8}x_{2,2} \\ &+ \frac{12-5\sqrt{3}}{5\sqrt{6}}x_{2,3} + \frac{2}{3\sqrt{8}}x_{2,4} + \frac{1}{3}x_{3,3} + \frac{24-7\sqrt{5}}{7\sqrt{12}}x_{3,4} \\ &+ \frac{32-8\sqrt{6}}{32}x_{4,4}. \end{aligned} \quad (3.2)$$

Now let \mathcal{T}'_{n,n_1} be the set of molecular trees with satisfy

$$x_{1,4} = n_1,$$

$$x_{2,2} = n - 2n_1 + 3,$$

$$x_{2,4} = n_1 - 4,$$

$$n_2 = n - \frac{3}{2}n_1 + 1,$$

$$n_3 = 0,$$

and

$$n_4 = \frac{1}{2}n_1 - 1.$$

Motivated by Theorem 3.1, we prove the following result.

Theorem 3.2. *Let T be a molecular tree with n vertices, $n_1 \geq 5$ of which are pendant vertices. Then*

$$(GA - ABC)(T) \geq \frac{2-\sqrt{2}}{2}n + \frac{35\sqrt{2}-15\sqrt{3}-30}{30}n_1 + \frac{18-13\sqrt{2}}{6},$$

with equality holds if and only if $T \in \mathcal{T}'_{n,n_1}$.

Proof. Since T is a molecular tree, we have (3.1). Suppose

$$f_1 = x_{1,2} + x_{1,3} + x_{1,4},$$

$$f_2 = x_{1,2} + x_{2,3},$$

$$f_3 = x_{1,3} + x_{2,3} + 2x_{3,3} + x_{3,4},$$

$$f_4 = x_{1,4} + x_{3,4} + 2x_{4,4},$$

that is,

$$f_1 = n_1,$$

$$f_2 = 2n_2 - 2x_{2,2} - x_{2,4},$$

$$f_3 = 3n_3,$$

$$f_4 = 4n_4 - x_{2,4},$$

we have

$$\sum_{i=1}^4 f_i = 2(n-1) - 2(x_{2,2} + x_{2,4}),$$

$$\sum_{i=1}^4 \frac{1}{i} f_i = n - (x_{2,2} + \frac{3}{4}x_{2,4}),$$

implying that

$$x_{2,2} = \frac{3}{2} \sum_{i=1}^4 f_i - 4 \sum_{i=1}^4 \frac{1}{i} f_i + n + 3,$$

$$x_{2,4} = -2 \sum_{i=1}^4 f_i + 4 \sum_{i=1}^4 \frac{1}{i} f_i - 4.$$

Thus we have

$$x_{1,4} = n_1 - x_{1,2} - x_{1,3},$$

$$x_{2,2} = n - 2n_1 + 3 - x_{1,2} - \frac{1}{3}x_{1,3} - \frac{1}{3}x_{2,3} + \frac{1}{3}x_{3,3} + \frac{2}{3}x_{3,4} + x_{4,4},$$

$$x_{2,4} = n_1 - 4 + x_{1,2} + \frac{1}{3}x_{1,3} - \frac{2}{3}x_{2,3} - \frac{4}{3}x_{3,3} - \frac{5}{3}x_{3,4} - 2x_{4,4}.$$

Substituting them back into (3.2), we have

$$\begin{aligned} (GA - ABC)(T) &= \frac{2 - \sqrt{2}}{2}n + \left[\frac{8 - 5\sqrt{3}}{10} - \left(\frac{8 - 4\sqrt{2}}{4} \right) + \frac{2}{3\sqrt{8}} \right] n_1 + \left(\frac{24 - 12\sqrt{2}}{8} - \frac{8}{3\sqrt{8}} \right) \\ &+ \left[\frac{1}{3\sqrt{2}} - \left(\frac{8 - 5\sqrt{3}}{10} \right) - \left(\frac{8 - 4\sqrt{2}}{8} \right) + \frac{2}{3\sqrt{8}} \right] x_{1,2} \\ &+ \left[\frac{6 - 4\sqrt{2}}{4\sqrt{3}} - \left(\frac{8 - 5\sqrt{3}}{10} \right) - \left(\frac{8 - 4\sqrt{2}}{24} \right) + \frac{2}{9\sqrt{8}} \right] x_{1,3} \\ &+ \left[\frac{4\sqrt{2} - 8}{24} + \frac{12 - 5\sqrt{3}}{5\sqrt{6}} - \frac{4}{9\sqrt{8}} \right] x_{2,3} + \left[\frac{8 - 4\sqrt{2}}{24} - \frac{8}{9\sqrt{8}} + \frac{1}{3} \right] x_{3,3} \\ &+ \left[\frac{16 - 8\sqrt{2}}{24} - \frac{10}{9\sqrt{8}} + \frac{24 - 7\sqrt{5}}{7\sqrt{12}} \right] x_{3,4} + \left[\frac{8 - 4\sqrt{2}}{8} - \frac{4}{3\sqrt{8}} + \frac{32 - 8\sqrt{6}}{32} \right] x_{4,4} \\ &= \frac{2 - \sqrt{2}}{2}n + \frac{35\sqrt{2} - 15\sqrt{3} - 30}{30}n_1 + \frac{18 - 13\sqrt{2}}{6} \\ &+ \frac{15\sqrt{3} + 25\sqrt{2} - 54}{30}x_{1,2} + \frac{45\sqrt{3} + 10\sqrt{2} - 15\sqrt{6} - 51}{45}x_{1,3} \\ &+ \frac{18\sqrt{6} - 20\sqrt{2} - 15}{45}x_{2,3} + \frac{12 - 7\sqrt{2}}{18}x_{3,3} \\ &+ \frac{84 + 72\sqrt{3} - 77\sqrt{2} - 21\sqrt{15}}{126}x_{3,4} + \frac{24 - 10\sqrt{2} - 3\sqrt{6}}{12}x_{4,4} \end{aligned}$$

$$\begin{aligned}
&= \frac{2 - \sqrt{2}}{2}n + \frac{35\sqrt{2} - 15\sqrt{3} - 30}{30}n_1 + \frac{18 - 13\sqrt{2}}{6} \\
&\quad + 0.244536705x_{1,2} + 0.096490573x_{1,3} + 0.017923202x_{2,3} \\
&\quad + 0.116694725x_{3,3} + 0.146671139x_{3,4} + 0.209116262x_{4,4},
\end{aligned}$$

with positive coefficients $x_{1,2}$, $x_{1,3}$, $x_{2,3}$, $x_{3,3}$, $x_{3,4}$ and $x_{4,4}$. Thus

$$(GA - ABC)(T) \geq \frac{2 - \sqrt{2}}{2}n + \frac{35\sqrt{2} - 15\sqrt{3} - 30}{30}n_1 + \frac{18 - 13\sqrt{2}}{6},$$

with equality holds if and only if the parameters $x_{1,2}$, $x_{1,3}$, $x_{2,3}$, $x_{3,3}$, $x_{3,4}$ and $x_{4,4}$ are all equal to zero, or equivalently, $x_{1,4} = n_1$, $x_{2,2} = n - 2n_1 + 3$, $x_{2,4} = n_1 - 4$, $n_2 = n - \frac{3}{2}n_1 + 1$, $n_3 = 0$ and $n_4 = \frac{1}{2}n_1 - 1$, i.e., $T \in \mathcal{T}'_{n,n_1}$. \square

4. Conclusions

In this paper, we characterized the first three minimum values of $GA - ABC$ index, where GA and ABC are the geometric-arithmetic index and atom-bond connectivity index, respectively. In particular, we characterized the first, the second and the third minimum n -vertex binary trees with respect to the invariant $GA - ABC$. We also obtained a sharp lower bound for the $GA - ABC$ index of molecular trees with fixed number of pendant vertices.

Acknowledgment

The authors would like to thank the anonymous referees for their valuable comments and constructive comments that improve the paper. This research is supported by the Research Intensified Grant Scheme (RIGS), Phase 1/2019, Universiti Malaysia Terengganu, Malaysia with Grant Vot. 55192/6.

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