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Research Article

Further Properties of Trees with Minimal Atom-Bond Connectivity Index

Jianping Liu and Jinsong Chen

College of Mathematics and Computer Science, Fuzhou University, Fuzhou 350116, China

Correspondence should be addressed to Jinsong Chen; fzu_cjs@126.com

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Let $G = (V, E)$ be a graph the atom-bond connectivity (ABC) index is defined as the sum of weights $((d_u + d_v - 2)/d_u d_v)^{1/2}$ over all edges uv of G, where d_u denotes the degree of a vertex u of G. In this paper, we determined a few structural features of the trees with minimal ABC index also we characterized the trees with $\text{dia}[T] = 2$ and minimal ABC index, where $[T]$ is induced by the vertices of degree greater than 2 in T and $\text{dia}[T]$ is the diameter of $[T]$.

1. Introduction

Let $G = (V, E)$ be a finite, simple, and undirected graph. The degree of a vertex $u \in V$ is denoted by d_u. The atom-bond connectivity (ABC) index is defined as the sum of weights $((d_u + d_v - 2)/d_u d_v)^{1/2}$ over all edges uv of G; that is,

$$\text{ABC}(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}. \quad (1)$$

The ABC index of a graph was defined by Estrada et al. [1] and it has many chemical applications [1, 2].

When examining a topological index, one of the fundamental questions that needs to be answered is for which graphs this index assumes minimal and maximal values and what are these extremal values. In the case of the ABC index, finding the tree for which this index is maximal was relatively easy [3]; it is the star. Eventually, also the trees with second-maximal, third-maximal, and so forth ABC index were determined [4].

We [5] have shown that by deleting an edge from any graph, the ABC index decreases. This result implies that among all n-vertex graphs, the complete graph K_n has maximal ABC value. Further, among all connected n-vertex graphs, minimal ABC is achieved by some tree. Thus the n-vertex trees with minimal ABC index are also the n-vertex connected graphs with minimal ABC index. But the problem of characterizing the n-vertex trees with minimal ABC index turned out to be much more difficult, and a complete solution of this problem is not known. For more results on ABC index see [6–13].

In a recent work [6] a combination of computer search and mathematical analysis was undertaken, aimed at elucidating the structure of the minimal ABC trees. And some structural features of the trees with minimal ABC index are given in [7].

Lemma 1 (see [6]). *If $n \geq 10$, then the n-vertex tree with minimal ABC index contains at most one pendent path of length $k = 3$.*

Lemma 2 (see [7]). *If $n \geq 10$, then each pendent vertex of the n-vertex tree G with minimal ABC index belongs to a pendent path of length k, $2 \leq k \leq 3$.*

By inspecting the structural features of these trees, in [8] the branches $B_1, \ldots, B_5$ and B_3^* were given. Let B_i be a branch of tree T formed by attaching i pendant path of length 2 to the vertex v such that the degree of v in T is $i + 1$. Let B_i^* be a branch of tree T formed by attaching $i - 1$ pendant path of length 2 and a pendant path of length 3 to the vertex v such that the degree of v in T is $i + 1$ (see Figure 1). Denote by kB_i the k union of the branches B_i and by $N(B_i)$ the number of

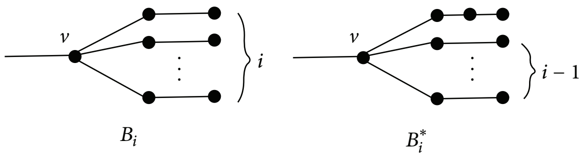


FIGURE 1: The branches B_i and B_i^*.

branches B_i in T. From Lemmas 1 and 2, we know all branches in a tree T with minimal ABC index must be of the type B_i or B_i^*, and $N(B_i^*) \leq 1, i = 1, 2, \ldots$. According to Lemma 1, in the following we assume that $N(B_3^*) \leq 1$ and $N(B_i^*) = 0$, for all $i \neq 3$.

In [9] the n-vertex minimal ABC trees were determined up to $n = 300$ and then a conjecture about the trees with minimal ABC index was presented.

Conjecture 3 (see [9]). *Let G be a tree with minimal ABC index among all trees of size n. Let T_0, T_1, T_2, T_3, T_4, T_5, and T_6 be the structures depicted in Figure 2.*

(i) *If $n \equiv 0 \pmod 7$, $n \geq 175$ and $n = 7k + 28$, then G has the structure T_0.*

(ii) *If $n \equiv 1 \pmod 7$, $n \geq 64$ and $n = 7k + 1$, then G has the structure T_1.*

(iii) *If $n \equiv 2 \pmod 7$, $n \geq 1185$ and $n = 7k + 9$, then G has the structure T_2.*

(iv) *If $n \equiv 3 \pmod 7$, $n \geq 80$ and $n = 7k + 10$, then G has the structure T_3.*

(v) *If $n \equiv 4 \pmod 7$, $n \geq 312$ and $n = 7k + 11$, then G has the structure T_4.*

(vi) *If $n \equiv 5 \pmod 7$, $n \geq 117$ and $n = 7k + 19$, then G has the structure T_5.*

(vii) *If $n \equiv 6 \pmod 7$, $n \geq 62$ and $n = 7k + 6$, then G has the structure T_6.*

In this paper, we determined a few structural features of the trees with minimal ABC index, also we characterized the trees with dia$[T] = 2$ and minimal ABC index, where dia$[T]$ is the diameter of $[T]$, which was induced by the vertices of degree greater than 2 in T.

2. The Structural Features of the Trees with Minimal ABC Index

Now, we are going to determine a few structural features of the trees with minimal ABC index.

Theorem 4. *The n-vertex tree with minimal ABC index does not contain branches B_k and B_k^* $(k \geq 6)$.*

Proof. Suppose that T_k^1 is a tree with minimal ABC index, possessing a branch B_k, $k \geq 6$. Let u be a vertex of T_k^1, adjacent to the vertex v, and the degree of u is s. Consider the tree T_k^2 (see Figure 3).

By direct calculation, we have

$$\mathrm{ABC}\left(T_k^1\right) - \mathrm{ABC}\left(T_k^2\right) = \sqrt{\frac{k+s-1}{(k+1)s}} + \sqrt{2} - \sqrt{\frac{k+s-4}{(k-2)s}} - 2\sqrt{\frac{k-1}{3(k-2)}}. \quad (2)$$

If $k = 6$, it can be easily checked by computer that

$$\sqrt{\frac{s+5}{7s}} + \sqrt{2} - \sqrt{\frac{s+2}{4s}} - 2\sqrt{\frac{5}{12}} > 0, \quad \text{that is,} \quad \mathrm{ABC}\left(T_k^1\right) > \mathrm{ABC}\left(T_k^2\right). \quad (3)$$

For the case $k \geq 7$, if the inequality $\mathrm{ABC}(T_k^1) > \mathrm{ABC}(T_k^2)$ holds, it implies that

$$\frac{k+s-1}{(k+1)s} + 2 + 2\sqrt{\frac{2k+2s-2}{(k+1)s}} > \frac{k+s-4}{(k-2)s} + \frac{4(k-1)}{3(k-2)} + \frac{4\sqrt{(k-1)(k+s-4)}}{(k-2)\sqrt{3s}}. \quad (4)$$

By elementary calculation, this inequality can be transformed to

$$3(k-2)(k+s-1) + 6s(k+1)(k-2) - 3(k+1)(k+s-4) - 4s(k+1)(k-1) > 4(k+1)\sqrt{3s(k-1)(k+s-4)} - 6(k-2)\sqrt{s(k+1)(2k+2s-2)}. \quad (5)$$

That is,

$$2k^2s - 6ks - 17s + 18 + 6(k-2) \times \sqrt{s(k+1)(2k+2s-2)} > 4(k+1)\sqrt{3s(k-1)(k+s-4)}. \quad (6)$$

By squaring the above relation and rearranging, we get

$$\left(4k^4s^2 - 196k^2s^2\right) + \left(252ks^2 - 1092s\right) + \left(24k^4s - 144k^3s\right) + \left(528k^2s - 72ks\right) + 625s^2 + 324 + \left(12\sqrt{2}(k-2)\left(2k^2s - 6ks - 17s + 18\right) \times\sqrt{(k+1)s(k+s-1)} - 100k^2s^2\right) > 0. \quad (7)$$

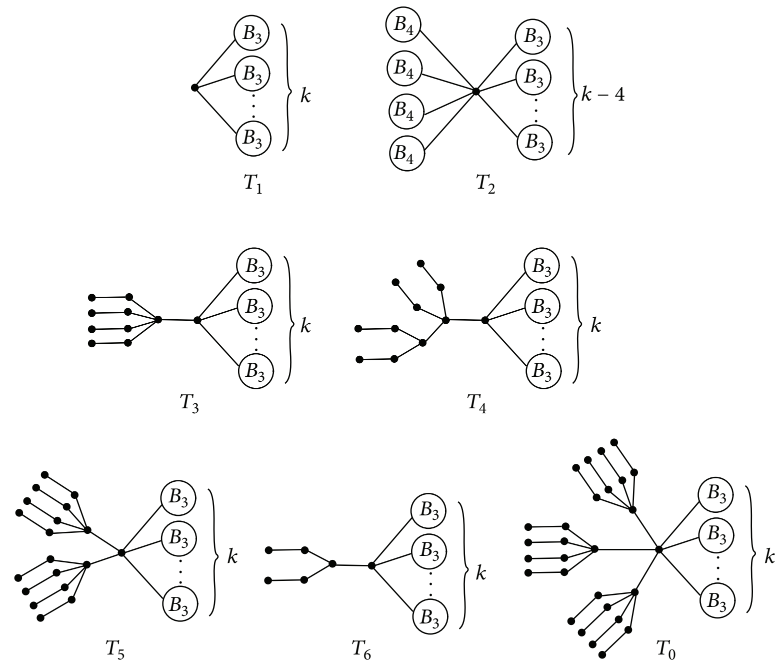


Figure 2: Types of trees with minimal ABC index correspond to Conjecture 3.

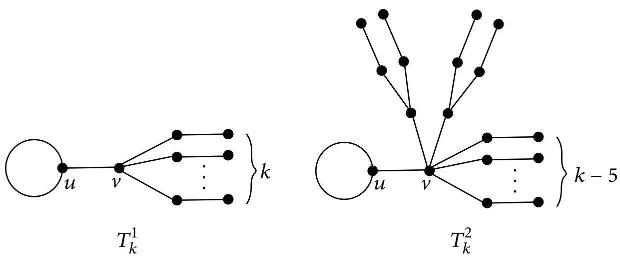


Figure 3

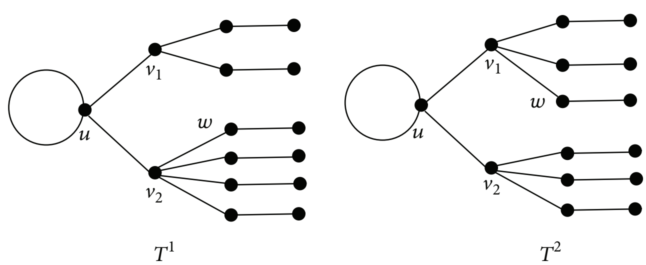


Figure 4

Since the function

$$\begin{aligned} g(k,s) &= 12\sqrt{2}(k-2)\left(2k^2s-6ks-17s+18\right) \\ &\quad\times\sqrt{(k+1)s(k+s-1)}-100k^2s^2. \\ &> 16(k-2)\left(2k^2-6k-17\right) \\ &\quad\times\sqrt{k+1}s^2-100k^2s^2>0 \quad (\text{as } k\geq 7, s\geq 3), \end{aligned} \tag{8}$$

and it holds that

$$\begin{gathered} 4k^4s^2-196k^2s^2>0, \\ 252ks^2-1092s>0, \\ 24k^4s-144k^3s>0, \\ 528k^2s-72ks>0 \quad (\text{as } k\geq 7, s\geq 3), \end{gathered} \tag{9}$$

thus, we have

$$\mathrm{ABC}\left(T_k^1\right)>\mathrm{ABC}\left(T_k^2\right), \quad \text{for } k\geq 7. \tag{10}$$

In the same way, we can prove that the n-vertex tree with minimal ABC index does not contain branch B_k^* $(k\geq 6)$.

The proof is complete. □

Note that Theorem 4 holds for all n-vertex trees with minimal ABC index.

Theorem 5. *Let T be a tree with minimal ABC index, then every vertex of T must not be connected with both B_2 and B_4.*

Proof. Suppose that T^1 is a tree with minimal ABC index; let u be a vertex of T^1, which is connected with both B_2 and B_4, and the degree of u is s $(s\geq 3)$. Construct the tree T^2 by deleting the edge v_2w and connecting w with v_1 (see Figure 4).

The transformation $T^1 \rightarrow T^2$ causes the following change of the ABC index:

$$\mathrm{ABC}\left(T^1\right) - \mathrm{ABC}\left(T^2\right) = \sqrt{\frac{s+3}{5s}} + \sqrt{\frac{s+1}{3s}} - 2\sqrt{\frac{s+2}{4s}}. \tag{11}$$

If the inequality $\mathrm{ABC}(T^1) > \mathrm{ABC}(T^2)$ holds, it implies that

$$\frac{s+3}{5s} + \frac{s+1}{3s} + 2\sqrt{\frac{(s+1)(s+3)}{15s^2}} > \frac{s+2}{s}. \tag{12}$$

By elementary calculation, this inequality can be transformed to

$$11s^2 + 16s - 76 > 0 \quad (s \geq 3). \tag{13}$$

Thus we have $\mathrm{ABC}(T^1) > \mathrm{ABC}(T^2)$, for $s \geq 3$.

The proof is complete. □

Theorem 6. *Let T be a tree with minimal ABC index; then every vertex of T must not be connected with both B_1 and $2B_4$.*

Proof. Suppose that T^3 is a tree with minimal ABC index; let u be a vertex of T^3, which is connected with both B_1 and $2B_4$, and the degree of u is s (obviously $s \geq 3$). Construct the tree T^4 by deleting the edges v_2w_2, v_3w_3 and adding the edges w_1w_2, v_1w_3 (see Figure 5).

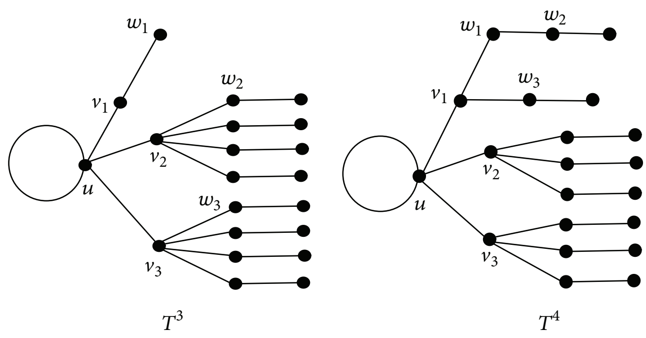


Figure 5

The transformation $T^3 \rightarrow T^4$ causes the following change of the ABC index:

$$\mathrm{ABC}\left(T^3\right) - \mathrm{ABC}\left(T^4\right) = \frac{\sqrt{2}}{2} + 2\sqrt{\frac{s+3}{5s}} - \sqrt{\frac{s+1}{3s}} - 2\sqrt{\frac{s+2}{4s}}. \tag{14}$$

If the inequality $\mathrm{ABC}(T^3) > \mathrm{ABC}(T^4)$ holds, it implies that

$$\frac{1}{2} + \frac{4(s+3)}{5s} + 2\sqrt{\frac{2(s+3)}{5s}} > \frac{4s+7}{3s} + \frac{2}{s}\sqrt{\frac{s^2+3s+2}{3}}. \tag{15}$$

That is

$$\frac{1}{2} + \frac{4(s+3)}{5s} + 2\sqrt{\frac{2(s+3)}{5s}} - \frac{4s+7}{3s} > \frac{2}{s}\sqrt{\frac{s^2+3s+2}{3}}. \tag{16}$$

By squaring the above relation and rearranging, we get

$$\frac{(s-2)\left(1198 + \left(241 - 24\sqrt{(10s+30)/s}\right)s\right)}{900s^2} > 0 \quad (s \geq 3). \tag{17}$$

Thus we have $\mathrm{ABC}(T^3) > \mathrm{ABC}(T^4)$, for $s \geq 3$, and the proof is complete. □

Theorem 7. *Let T be a tree with minimal ABC index; then every vertex of T must not be connected with $7B_4$.*

Proof. Suppose that T^7 is a tree with minimal ABC index, possessing a vertex u in T^7 connected with $7B_4$ (see Figure 6). Let $U = \{v_1, v_2, \ldots, v_s\}$ be the set of adjacent vertices to u. Let $d_1, d_2, \ldots, d_s$ be the degree of $v_1, v_2, \ldots, v_s$, respectively. We consider the tree T^8 shown in Figure 6.

Here we are going to show that $\mathrm{ABC}(T^7) - \mathrm{ABC}(T^8) > 0$, for any $s \geq 7$.

Consider

$$\begin{aligned}\mathrm{ABC}\left(T^7\right) - \mathrm{ABC}\left(T^8\right) &= 7\sqrt{\frac{s+3}{5s}} + \sqrt{2} - 9\sqrt{\frac{s+4}{4(s+2)}} \\ &\quad + \sum_{i=8}^{s}\left(\sqrt{\frac{s+d_i-2}{sd_i}} - \sqrt{\frac{s+d_i}{(s+2)d_i}}\right),\end{aligned} \tag{18}$$

for any $d_i \geq 2$, $\sqrt{(s+d_i-2)/(sd_i)} - \sqrt{(s+d_i)/((s+2)d_i)} > 0$.

Now we are going to show that $7\sqrt{(s+3)/(5s)} + \sqrt{2} > 9\sqrt{(s+4)/4(s+2)}$; that is

$$\frac{49(s+3)}{5s} + 2 + 14\sqrt{\frac{2(s+3)}{5s}} > \frac{81(s+4)}{4(s+2)}. \tag{19}$$

By elementary calculation, this inequality can be transformed to

$$2799s^4 + 30240s^3 + 585648s^2 + 1693440s - 1382976 > 0. \tag{20}$$

The largest root of the above polynomial is 0.660387; therefore, the value of the above polynomial is positive for $s > 0.660387$.

Thus we have $\mathrm{ABC}(T^7) > \mathrm{ABC}(T^8)$, and the proof is complete. □

Theorem 8. *Let T be a tree with minimal ABC index; then every vertex of T must not be connected with $2B_5$.*

Proof. Suppose that T_5^1 is a tree with minimal ABC index, possessing a vertex connected with $2B_5$. Let u be the vertex of T_5^1, adjacent to the vertices v_1 and v_2, and the degree of u is s ($s \geq 3$). Consider the tree T_5^2 (see Figure 7).

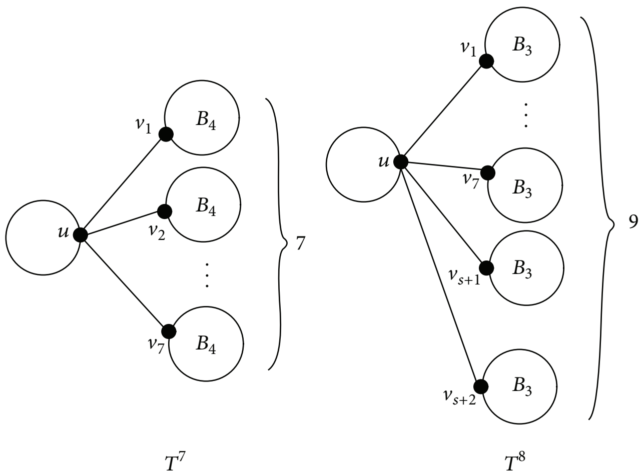


Figure 6

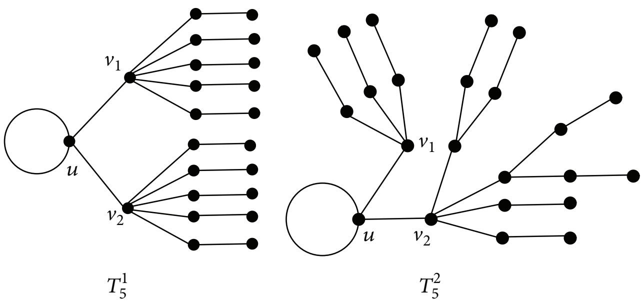


Figure 7

The transformation $T_5^1 \rightarrow T_5^2$ causes the following change of the ABC index:

$$\mathrm{ABC}\left(T_5^1\right) - \mathrm{ABC}\left(T_5^2\right) = 2\sqrt{\frac{s+4}{6s}} + \sqrt{2} - \sqrt{\frac{s+2}{4s}} - \sqrt{\frac{s+3}{5s}} - 2\sqrt{\frac{6}{15}}. \tag{21}$$

It can be easily checked by computer that $\mathrm{ABC}(T_5^1) > \mathrm{ABC}(T_5^2)$, for $s \geq 3$.

The proof is complete. □

3. The Minimal ABC Indices of Trees with Order n and $\mathrm{dia}[T] = 2$

Denote by $[T]$ the subgraph of T induced by its vertices of degree greater than 2. For a connected graph G, the diameter of G, denoted by dia$G$, is the length of a longest path of G.

Lemma 9 (see [7]). *Let T be an n-vertex ($n \geq 10$) tree with minimal ABC index; then $[T]$ is a tree.*

Note that the structures T_i in Conjecture 3 have $\mathrm{dia}[T_i] = 2$ ($i = 0, 1, 2, 3, 5, 6$). Let $T_{n,2}$ be the set of n-vertex trees T with $\mathrm{dia}[T] = 2$.

Now we will characterize the trees with $\mathrm{dia}[T] = 2$ and minimal ABC index, which partially solve Conjecture 3.

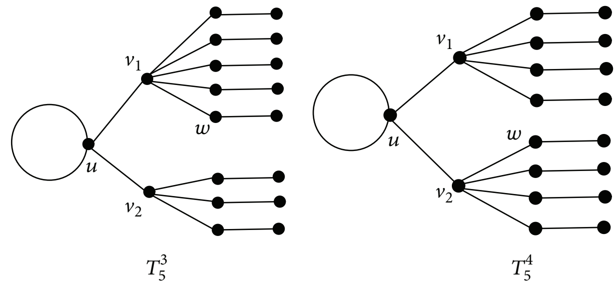


Figure 8

Lemma 10. *Let $T \in T_{n,2}$ be a tree with minimal ABC index; then T does not contain B_5.*

Proof. Let $T_5^3 \in T_{n,2}$ be a tree with minimal ABC index. By Theorems 7 and 8, T_5^3 contains at most $6B_4$, $1B_5$; hence, for $n > 65$, T_5^3 must contain B_3. Suppose that T_5^3 possesses B_5; then we can construct the tree T_5^4 by deleting the edge v_1w and adding the edge v_2w (see Figure 8).

The transformation $T_5^3 \rightarrow T_5^4$ causes the following change of the ABC index:

$$\mathrm{ABC}\left(T_5^3\right) - \mathrm{ABC}\left(T_5^4\right) = \sqrt{\frac{d_u+4}{6d_u}} + \sqrt{\frac{d_u+2}{4d_u}} - 2\sqrt{\frac{d_u+3}{5d_u}}. \tag{22}$$

It can be easily checked that $\mathrm{ABC}(T_5^3) > \mathrm{ABC}(T_5^4)$, for $d_u \geq 3$.

The proof is complete. □

Lemma 11. *Let $T \in T_{n,2}$ be a tree with minimal ABC index; if the maximum degree $\Delta \geq 24$, then T must not contain kB_2 ($k \geq 3$).*

Proof. Suppose that $T^5 \in T_{n,2}$ is a tree with minimal ABC index, possessing $3B_2$ (see Figure 9). Let u be the vertex with maximum degree of T^5, adjacent to the vertices v_1, v_2, and v_3, and the degree of u is $s+1$. Construct the tree T^6 by deleting the edges v_3w_1 and uv_3 and adding the edges v_1w_1 and v_2v_3. Let $U = \{v_1, v_2, \ldots, v_{s+1}\}$ be a set of adjacent vertices to u. Let $d_1, d_2, \ldots, d_{s+1}$ be the degree of $v_1, v_2, \ldots, v_{s+1}$, respectively.

The transformation $T^5 \rightarrow T^6$ causes the following change of the ABC index:

$$\mathrm{ABC}\left(T^5\right) - \mathrm{ABC}\left(T^6\right) = 3\sqrt{\frac{s+2}{3(s+1)}} - 2\sqrt{\frac{s+2}{4s}} - \frac{\sqrt{2}}{2} + \sum_{i=4}^{s+1}\left(\sqrt{\frac{s+d_i-1}{(s+1)d_i}} - \sqrt{\frac{s+d_i-2}{sd_i}}\right). \tag{23}$$

By Theorems 4 and 5, Lemma 10, and noticing that $T \in T_{n,2}$, we know that $d_i = 2, 3$ or 4.

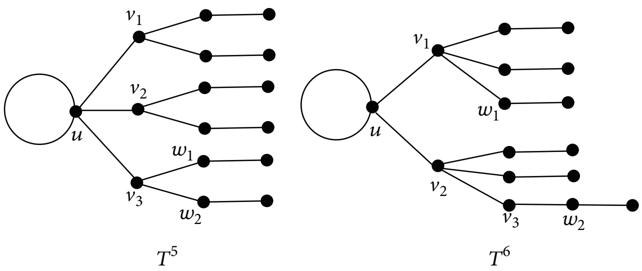


FIGURE 9

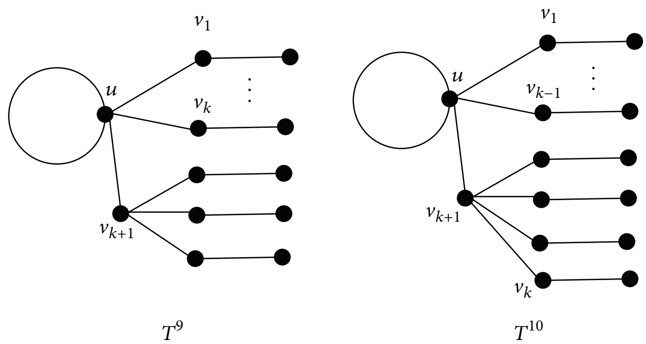


FIGURE 10

And consider

$$\sqrt{\frac{s+3}{4(s+1)}}-\sqrt{\frac{s+2}{4s}} = \min_{d_i=2,3,4}\left(\sqrt{\frac{s+d_i-1}{(s+1)d_i}}-\sqrt{\frac{s+d_i-2}{sd_i}}\right). \tag{24}$$

Putting this in the above expression, we get

$$\begin{aligned}\operatorname{ABC}\left(T^5\right)-\operatorname{ABC}\left(T^6\right) &\geq 3\sqrt{\frac{s+2}{3(s+1)}}-2\sqrt{\frac{s+2}{4s}}-\frac{\sqrt{2}}{2} \\ &\quad + (s-2)\left(\sqrt{\frac{s+3}{4(s+1)}}-\sqrt{\frac{s+2}{4s}}\right) \\ &= 3\sqrt{\frac{s+2}{3(s+1)}}+(s-2)\sqrt{\frac{s+3}{4(s+1)}}-\left(\frac{s}{2}\sqrt{\frac{s+2}{s}}+\frac{\sqrt{2}}{2}\right).\end{aligned} \tag{25}$$

If the inequality $\operatorname{ABC}(T^5)>\operatorname{ABC}(T^6)$ holds, it implies that

$$\frac{3(s+2)}{s+1}+\frac{(s-2)^2(s+3)}{4(s+1)}+\frac{s-2}{s+1}\sqrt{3(s+2)(s+3)} > \frac{s(s+2)}{4}+\frac{1}{2}+\sqrt{\frac{s(s+2)}{2}}. \tag{26}$$

By elementary calculation, this inequality can be transformed to

$$2(s-2)\sqrt{3(s+2)(s+3)} > 2s^2-17+(s+1)\sqrt{2s(s+2)}. \tag{27}$$

By squaring the above relation and rearranging for two times, we get

$$s^8-20s^7-86s^6+248s^5+956s^4-430s^3 -2183s^2-1130s+\frac{1}{4}>0. \tag{28}$$

The largest root of the above polynomial is 23.1742; therefore, the value of the above polynomial is positive for $s>23.1742$. Thus we have $\operatorname{ABC}(T^5)>\operatorname{ABC}(T^6)$ for $s\geq 24$, and the proof is complete. □

Lemma 12. *Let $T\in T_{n,2}$ be a tree with minimal ABC index; if the maximum degree $\Delta\geq 13$, then T must not contain B_1.*

Proof. Suppose that $T^9\in T_{n,2}$ is a tree with maximum degree $\Delta\geq 13$ and minimal ABC index, possessing kB_1 $(k\geq 1)$ (see Figure 10). By Theorem 6 and Lemma 11, we have $N(B_2)\leq 2$ and $N(B_4)\leq 1$. Thus B_3 in T^9 must be contained.

Let u be the vertex with maximum degree s in T^9 and let $U=\{v_1,v_2,\ldots,v_s\}$ be a set of adjacent vertices to u. Let $d_1,d_2,\ldots,d_s$ be the degree of $v_1,v_2,\ldots,v_s$, respectively. Since $T^9\in T_{n,2}$ and by Theorem 4 and Lemma 10, we have $d_i=2,3,4$, or 5. Construct the tree T^{10} by deleting the edge uv_k and adding the edge $v_{k+1}v_k$ to T^9.

The transformation $T^9\to T^{10}$ causes the following change of the ABC index:

$$\begin{aligned}\operatorname{ABC}\left(T^9\right)-\operatorname{ABC}\left(T^{10}\right) &= \sum_{i=k+2}^{s}\left(\sqrt{\frac{d_i+s-2}{d_is}}-\sqrt{\frac{d_i+s-3}{d_i(s-1)}}\right) \\ &\quad +\left(\sqrt{\frac{s+2}{4s}}-\sqrt{\frac{s+2}{5(s-1)}}\right) \\ &= N(B_2)\left(\sqrt{\frac{s+1}{3s}}-\sqrt{\frac{s}{3(s-1)}}\right) \\ &\quad + N(B_4)\left(\sqrt{\frac{s+3}{5s}}-\sqrt{\frac{s+2}{5(s-1)}}\right) \\ &\quad + (s-k-1-N(B_2)-N(B_4)) \\ &\quad \times\left(\sqrt{\frac{s+2}{4s}}-\sqrt{\frac{s+1}{4(s-1)}}\right)+\left(\sqrt{\frac{s+2}{4s}}-\sqrt{\frac{s+2}{5(s-1)}}\right).\end{aligned} \tag{29}$$

If the inequality $\mathrm{ABC}(T^9) > \mathrm{ABC}(T^{10})$ holds, it implies that

$$\begin{aligned}
&\sqrt{\frac{s+2}{4s}}-\sqrt{\frac{s+2}{5(s-1)}} \\
&> N(B_2)\left(\sqrt{\frac{s}{3(s-1)}}-\sqrt{\frac{s+1}{3s}}\right) \\
&+ N(B_4)\left(\sqrt{\frac{s+2}{5(s-1)}}-\sqrt{\frac{s+3}{5s}}\right) \\
&+ (s-k-1-N(B_2)-N(B_4)) \\
&\times\left(\sqrt{\frac{s+1}{4(s-1)}}-\sqrt{\frac{s+2}{4s}}\right) \triangleq f(s,k).
\end{aligned} \tag{30}$$

Note that $N(B_2) \le 2$, $N(B_4) \le 1$, $k \ge 1$, and

$$\begin{aligned}
\sqrt{\frac{s}{3(s-1)}}-\sqrt{\frac{s+1}{3s}} &< \sqrt{\frac{s+1}{4(s-1)}}-\sqrt{\frac{s+2}{4s}} \\
&< \sqrt{\frac{s+2}{5(s-1)}}-\sqrt{\frac{s+3}{5s}}.
\end{aligned} \tag{31}$$

We have, $f(s,k) \le (\sqrt{(s+2)/(5(s-1))}-\sqrt{(s+3)/(5s)})+(s-3)(\sqrt{(s+1)/(4(s-1))}-\sqrt{(s+2)/(4s)})$.

Now we are going to show that

$$\begin{aligned}
\sqrt{\frac{s+2}{4s}}-\sqrt{\frac{s+2}{5(s-1)}} &> \left(\sqrt{\frac{s+2}{5(s-1)}}-\sqrt{\frac{s+3}{5s}}\right) \\
&+ (s-3)\left(\sqrt{\frac{s+1}{4(s-1)}}-\sqrt{\frac{s+2}{4s}}\right).
\end{aligned} \tag{32}$$

That is,

$$(s-2)\sqrt{\frac{s+2}{4s}}-2\sqrt{\frac{s+2}{5(s-1)}} > (s-3)\sqrt{\frac{s+1}{4(s-1)}}-\sqrt{\frac{s+3}{5s}}. \tag{33}$$

By squaring the above relation and rearranging for two times, we get

$$\begin{aligned}
&8\sqrt{5}(s-3)(5s-4)\left(2s^2-s+7\right)\sqrt{s(s-1)(s+1)(s+3)} \\
&\quad > 140s^6+180s^5-2709s^4+1734s^3 \\
&\qquad + 2151s^2-776s-784.
\end{aligned} \tag{34}$$

Since $\sqrt{s(s-1)(s+1)(s+3)} > (s+0.6)^2$ (for $s \ge 7$) and the largest root of the following polynomial is 12.9172,

$$\begin{aligned}
&8\sqrt{5}(s-3)(5s-4)\left(2s^2-s+7\right)(s+0.6)^2 \\
&\quad - 140s^6-180s^5+2709s^4-1734s^3 \\
&\quad - 2151s^2+776s+784 \\
&= 0.
\end{aligned} \tag{35}$$

Therefore the value of the above polynomial is positive for $s > 12.9172$. Thus we have $\mathrm{ABC}(T^9) > \mathrm{ABC}(T^{10})$ for $s \ge 13$ and the proof is complete. □

Theorem 13. *Let $T \in T_{n,2}$ be a tree with minimal ABC index and the maximum degree $\Delta \ge 24$. Let T_0, T_1, T_2, T_3, T_5, and T_6 be the structures depicted in Figure 2.*

(i) *If $n \equiv 0 \pmod 7$, $n \ge 175$ and $n = 7k+28$, then T has the structure T_0.*

(ii) *If $n \equiv 1 \pmod 7$, $n \ge 169$ and $n = 7k+1$, then T has the structure T_1.*

(iii) *If $n \equiv 2 \pmod 7$, $n \ge 1185$ and $n = 7k+9$, then T has the structure T_2.*

(iv) *If $n \equiv 3 \pmod 7$, $n \ge 171$ and $n = 7k+10$, then T has the structure T_3.*

(v) *If $n \equiv 4 \pmod 7$, $n \ge 2020$ and $n = 7k+11$, then T has the structure T_4' depicted in Figure 11(b).*

(vi) *If $n \equiv 5 \pmod 7$, $n \ge 173$ and $n = 7k+19$, then T has the structure T_5.*

(vii) *If $n \equiv 6 \pmod 7$, $n \ge 167$ and $n = 7k+6$, then T has the structure T_6.*

Proof. Let $T \in T_{n,2}$ be a tree with minimal ABC index. From Lemmas 1 and 2, we know all branches of T must be of the type B_i or B_i^*, $i = 1, 2, \ldots$. And from Theorem 4 and Lemmas 10 and 12, we know all branches of T must be of the type B_i or B_i^*, $i = 2, 3, 4$.

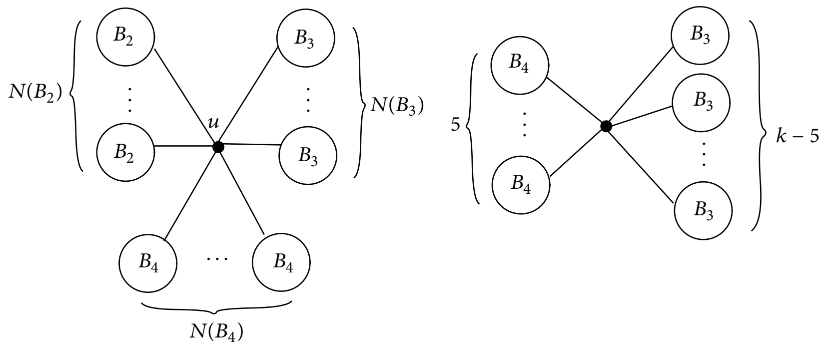
Then the minimal ABC tree $T \in T_{n,2}$ has

$$n = 1 + 5N(B_2) + 7N(B_3) + 9N(B_4) + x \tag{36}$$

vertices, where $x \in \{0, 1\}$ counts the pendent paths of length 3.

From above we see that the tree $T \in T_{n,2}$ with minimal ABC index and $x = 0$ must possess the structure as shown in Figure 11(a). It is easy to see that

$$\begin{aligned}
&\mathrm{ABC}(T) \\
&= N(B_2)\sqrt{\frac{d_u+1}{3d_u}} + N(B_3)\sqrt{\frac{d_u+2}{4d_u}} + N(B_4)\sqrt{\frac{d_u+3}{5d_u}} \\
&\quad + (n-1-N(B_2)-N(B_3)-N(B_4))\frac{\sqrt{2}}{2}.
\end{aligned} \tag{37}$$



(a) The minimal ABC tree T in $T_{n,2}$ (b) $T_4{}'$

Figure 11

Putting (36) in the above equation, we have

$$\begin{aligned} f(D) &\triangleq \mathrm{ABC}(T) \\ &= N(B_2)\sqrt{\frac{d_u+1}{3d_u}} + N(B_3)\sqrt{\frac{d_u+2}{4d_u}} \\ &\quad + N(B_4)\sqrt{\frac{d_u+3}{5d_u}} + (4N(B_2) + 6N(B_3) \\ &\qquad + 8N(B_4) + x)\frac{\sqrt{2}}{2}, \end{aligned} \tag{38}$$

where $d_u = \Delta = N(B_2) + N(B_3) + N(B_4)$ and $D = (N(B_2), N(B_3), N(B_4), x)$.

From Lemma 11 and Theorems 5 and 7, we get

$$\begin{gathered} N(B_2) \in \{0,1,2\},\quad N(B_4) \in \{0,1,2,3,4,5,6\}, \\ N(B_2)N(B_4) = 0. \end{gathered} \tag{39}$$

Note that the parameters n, $N(B_2)$, $N(B_3)$, $N(B_4)$, and x in (36) are nonnegative integers.

Consider

(i) $n \equiv 0 \pmod 7$ and $n = 7k + 28$.

Case 1.1. If $N(B_2) = 0$, then $n = 1 + 7N(B_3) + 9N(B_4) + x \equiv 0 \pmod 7$.

Thus, $9N(B_4) + x + 1 \equiv 0 \pmod 7$, we get $N(B_4) = 3$, $x = 0$ or $N(B_4) = 6$, $x = 1$.

That is, $D = (0, (n/7) - 4, 3, 0) = (0, k, 3, 0)$ or $(0, (n/7) - 8, 6, 1) = (0, k - 4, 6, 1)$.

Case 1.2. If $N(B_2) = 1$, then $N(B_4) = 0$, $n = 1 + 5 + 7N(B_3) + x \equiv 0 \pmod 7$; we get $x = 1$.

That is, $D = (1, (n/7) - 1, 0, 1) = (1, k + 3, 0, 1)$.

Case 1.3. If $N(B_2) = 2$, then $N(B_4) = 0$ and $n = 11 + 7N(B_3) + x \equiv 0 \pmod 7$; there is no solution.

Comparing the values $f(0, k, 3, 0)$, $f(0, k - 4, 6, 1)$, and $f(1, k + 3, 0, 1)$ and noting that $\Delta \ge 24$, we get that

$$f(0,k,3,0) = k\sqrt{\frac{k+5}{4(k+3)}} + 3\sqrt{\frac{k+6}{5(k+3)}} + (3k+12)\sqrt{2} \tag{40}$$

is the smallest one ($k \ge 21$); the result (i) follows.

Consider

(ii) $n \equiv 1 \pmod 7$ and $n = 7k + 1$.

Case 2.1. If $N(B_2) = 0$, then $9N(B_4) + x + 1 \equiv 1 \pmod 7$.

We get $N(B_4) = 0$, $x = 0$ or $N(B_4) = 3$, $x = 1$.

That is, $D = (0, k, 0, 0)$ or $(0, k - 4, 3, 1)$.

Case 2.2. If $N(B_2) = 1$, then $N(B_4) = 0$ and $n = 1 + 5 + 7N(B_3) + x$.

Thus $5 + x \equiv 0 \pmod 7$; there is no solution.

Case 2.3. If $N(B_3) = 2$, then $N(B_4) = 0$ and $n = 1 + 10 + 7N(B_3) + x$.

Thus $10 + x \equiv 0 \pmod 7$; there is no solution.

Comparing the values $f(0, k, 0, 0)$, $f(0, k - 4, 3, 1)$, we get that

$$f(0,k,0,0) = k\sqrt{\frac{k+2}{4k}} + 3k\sqrt{2} \tag{41}$$

is the smallest one ($k \ge 24$); the result (ii) follows.

Consider

(iii) $n \equiv 2 \pmod 7$ and $n = 7k + 9$.

Case 3.1. If $N(B_2) = 0$, then $n = 1 + 7N(B_3) + 9N(B_4) + x \equiv 2 \pmod 7$.

We get $N(B_4) = 0$, $x = 1$ or $N(B_4) = 4$, $x = 0$.

That is, $D = (0, k + 1, 0, 1)$ or $(0, k - 4, 4, 0)$.

Case 3.2. If $N(B_2) = 1$, then $N(B_4) = 0$ and $n = 1 + 5 + 7N(B_3) + x$.

Thus $6 + x \equiv 2 \pmod 7$; there is no solution.

Case 3.3. If $N(B_2) = 2$, then $N(B_4) = 0$ and $n = 1 + 10 + 7N(B_3) + x$.

Thus $11 + x \equiv 2 \pmod 7$; there is no solution.

Comparing the values $f(0, k+1, 0, 1)$, $f(0, k-4, 4, 0)$, we get that

$$f(0, k-4, 4, 0) = (k-4)\sqrt{\frac{k+2}{4k}} + 4\sqrt{\frac{k+3}{5k}} + (3k+4)\sqrt{2} \quad (42)$$

is the smallest one ($k \geq 168$); the result (iii) follows.

Consider

(iv) $n \equiv 3 \pmod 7$ and $n = 7k + 10$.

Case 4.1. If $N(B_2) = 0$, then $n = 1 + 7N(B_3) + 9N(B_4) + x \equiv 3 \pmod 7$.

We get $N(B_4) = 1$, $x = 0$ or $N(B_4) = 4$, $x = 1$.

That is, $D = (0, k, 1, 0)$ or $(0, k-4, 4, 1)$.

Case 4.2. If $N(B_2) = 1$, then $N(B_4) = 0$ and $n = 1 + 5 + 7N(B_3) + x$.

Thus $6 + x \equiv 3 \pmod 7$; there is no solution.

Case 4.3. If $N(B_2) = 2$, then $N(B_4) = 0$ and $n = 1 + 10 + 7N(B_3) + x$.

Thus $11 + x \equiv 3 \pmod 7$; there is no solution.

Comparing the values $f(0, k, 1, 0)$, $f(0, k-4, 4, 1)$, we get that

$$f(0, k, 1, 0) = k\sqrt{\frac{k+3}{4(k+1)}} + \sqrt{\frac{k+4}{5(k+1)}} + (3k+4)\sqrt{2} \quad (43)$$

is the smallest one ($k \geq 23$); the result (iv) follows.

Consider

(v) $n \equiv 4 \pmod 7$ and $n = 7k + 11$.

Case 5.1. If $N(B_2) = 0$, then $n = 1 + 7N(B_3) + 9N(B_4) + x \equiv 4 \pmod 7$.

We get $N(B_4) = 1$, $x = 1$ or $N(B_4) = 5$, $x = 0$.

That is, $D = (0, k, 1, 1)$ or $(0, k-5, 5, 0)$.

Case 5.2. If $N(B_2) = 1$, then $N(B_4) = 0$, $n = 1+5+7N(B_3)+x$.

Thus $6 + x \equiv 4 \pmod 7$; there is no solution.

Case 5.3. If $N(B_2) = 2$, then $N(B_4) = 0$ and $n = 1 + 10 + 7N(B_3) + x$.

Thus $11 + x \equiv 4 \pmod 7$, we get $x = 0$.

That is, $D = (2, k, 0, 0)$.

Comparing the values $f(0, k, 1, 1)$, $f(0, k-5, 5, 0)$, and $f(2, k, 0, 0)$, we get that

$$f(2, k, 0, 0) = k\sqrt{\frac{k+4}{4(k+2)}} + 2\sqrt{\frac{k+3}{3(k+2)}} + (3k+4)\sqrt{2} \quad (44)$$

is the smallest one ($k = 22, 23, \ldots, 286$) and that

$$f(0, k-5, 5, 0) = (k-5)\sqrt{\frac{k+2}{4k}} + 5\sqrt{\frac{k+3}{5k}} + (3k+5)\sqrt{2} \quad (45)$$

is the smallest one ($k \geq 287$). The result (v) follows.

Consider

(vi) $n \equiv 5 \pmod 7$ and $n = 7k + 19$.

Case 6.1. If $N(B_2) = 0$, then $n = 1 + 7N(B_3) + 9N(B_4) + x \equiv 5 \pmod 7$.

We get $N(B_4) = 2$, $x = 0$ or $N(B_4) = 5$, $x = 1$.

That is, $D = (0, k, 2, 0)$ or $(0, k-4, 5, 1)$.

Case 6.2. If $N(B_2) = 1$, then $N(B_4) = 0$ and $n = 1 + 5 + 7N(B_3) + x$.

Thus $6 + x \equiv 5 \pmod 7$; there is no solution.

Case 6.3. If $N(B_2) = 2$, then $N(B_4) = 0$ and $n = 1 + 10 + 7N(B_3) + x$.

Thus $11 + x \equiv 5 \pmod 7$, we get $x = 1$.

That is, $D = (2, k+1, 0, 1)$.

Comparing the values $f(0, k, 2, 0)$, $f(0, k-4, 5, 1)$, and $f(2, k+1, 0, 1)$, we get that

$$f(0, k, 2, 0) = k\sqrt{\frac{k+4}{4(k+2)}} + 2\sqrt{\frac{k+5}{5(k+2)}} + (3k+8)\sqrt{2} \quad (46)$$

is the smallest one ($k \geq 22$); the result (vi) follows.

Consider

(vii) $n \equiv 6 \pmod 7$ and $n = 7k + 6$.

Case 7.1. If $N(B_2) = 0$, then $n = 1 + 7N(B_3) + 9N(B_4) + x \equiv 6 \pmod 7$.

We get $N(B_4) = 2$, $x = 1$ or $N(B_4) = 6$, $x = 0$.

That is, $D = (0, k-2, 2, 1)$ or $(0, k-7, 6, 0)$.

Case 7.2. If $N(B_2) = 1$, then $N(B_4) = 0$ and $n = 1 + 5 + 7N(B_3) + x$.

Thus $6 + x \equiv 6 \pmod 7$, we get $x = 0$.

That is, $D = (1, k, 0, 0)$.

Case 7.3. If $N(B_2) = 2$, then $N(B_4) = 0$ and $n = 1 + 10 + 7N(B_3) + x$.

Thus $11 + x \equiv 6 \pmod 7$; there is no solution.

Comparing the values $f(0, k-2, 2, 1)$, $f(0, k-7, 6, 0)$, and $f(1, k, 0, 0)$, we get that

$$f(1, k, 0, 0) = k\sqrt{\frac{k+3}{4(k+1)}} + \sqrt{\frac{k+2}{3(k+1)}} + (3k+2)\sqrt{2} \quad (47)$$

is the smallest one ($k \geq 23$); the result (vii) follows. □

In [13], the authors also gave a similar result as Theorem 13 (in [13], a tree $T \in T_{n,2}$ without pendent path of length 3 is called a proper Krag tree), but we do it independently and the methods are also different.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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