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Proving a Conjecture of Gutman Concerning Trees with Minimal *ABC* Index

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Abstract

The atom-bond connectivity (*ABC*) index of a graph $G=(V,E)$ is defined as $ABC(G)=\sum_{uv\in E}\sqrt{[d(u)+d(v)-2]/[d(u)d(v)]}$, where $d(u)$ denotes the degree of vertex u of G. This recently introduced molecular structure descriptor found interesting applications in the study of the thermodynamic stability of acyclic saturated hydrocarbons, and the strain energy of their cyclic congeners. In connection with this, one needs to know which trees have extremal *ABC* index. However, the problem of characterizing trees with minimal *ABC* index appears to be difficult. One approach to the problem is to determine their structural features as much as possible. Gutman et al. [*MATCH Comun. Math. Comput. Chem*. **67** (2012) 467] conjectured that each pendent vertex of a tree with minimal *ABC* index belongs to a pendent path of length 2 or 3. We prove this conjecture in the present paper.

1. Introduction and notations

Molecular descriptors have found a wide application in QSPR/QSAR studies [1]. One of the best known is the Randić index introduced in 1975 by Randić [2], who has shown that this index reflects molecular branching. However, many physic-chemical properties are dependent on factors different than branching. In order to take this into account but at the same time to keep the spirit of the Randić index, in 1998 Estrada et al. [3] proposed the *atom-bond connectivity index*.

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The (molecular) graph considered will be denoted by $G=(V,E)$, and its vertex and edge sets by V and E, respectively. If $|V|=n$, then G is said to be an n-vertex graph. The 1-vertex graph is said to be *trivial*.

If u and v are two adjacent vertices of G, then the edge connecting them will be denoted by uv. If $uv \in E$, then we say v is a neighbor of u (in G). Let $N(u)$ denotes the set of the neighbors of u (in G).

If $uv \in E$, then $G-uv$ will denote the graph obtained from G by deleting the edge uv. If, in turn, $uv \notin E$, then $G+uv$ will denote the graph obtained from G by adding the edge uv.

For $u \in V$, $d(u)=|N(u)|$ is called the degree of vertex u. A vertex of degree 1 is said to be pendent. A pendent vertex is said to be of *star-type* if it is adjacent to a vertex of degree greater than 2. In particular, if G is a tree, then its pendent vertices are also called the leaves of G, and its vertices of degree greater than 1 are called the branching vertices of G. In addition, we will denote by $[T]$ the subgraph of a tree T induced by its vertices of degree greater than 2.

Let $P=u_0u_1\cdots u_{k-1}u_k$ be a path of length k in an n-vertex graph G with $d(u_0)\geq 3$ and $d(u_k)\neq 2$, where $1\leq k\leq n-1$. If $d(u_k)\geq 3$, then P is said to be an *internal path* of G. If $d(u_k)=1$, then P is said to be a *pendent path* (on u_0) of G.

Note that, a graph G contains no star-type pendent vertices iff G contains no pendent paths of length 1.

The atom-bond connectivity (*ABC*) index of a graph $G=(V,E)$ is defined as $ABC(G)=\sum_{uv\in E}\sqrt{[d(u)+d(v)-2]/[d(u)d(v)]}$.

Initially [3], the *ABC* index was shown to be well correlated with the heat of formation of alkanes, and that it thus can serve for predicting their thermodynamic properties, see also [4]. In addition to this, Estrada [5] elaborated a novel quantum-theory-like justification for this topological index, showing that it provides a model for taking into account 1,2-, 1,3-, and 1,4-interactions in the carbon-atom skeleton of saturated hydrocarbons, and that it can be used for rationalizing steric effects in such compounds. These results triggered a number of mathematical investigations of the *ABC* index [6-18].

Many studies focused on extremal *ABC* index values. For n-vertex trees, Furtula et al. [6] showed that the star S_n is the unique tree with maximal *ABC* index. Eventually, also the trees with second-maximal, third-maximal, etc. *ABC* index were determined [13]. However, the problem of characterizing n-vertex tree(s) with minimal ABC index appears to be difficult, and this task has not been completely solved until now. Recently, aided with computer searching, Gutman et al. [16] determined the n-vertex trees with minimal ABC index for $7 \leq n \leq 30$, and for $31 \leq n \leq 700$, the n-vertex trees with a single high-degree vertex, special branches, and minimal ABC index were also determined [18]. Gutman et al. [16] determined some structural features of trees with minimal ABC index (see Section 3), and proposed the following conjecture.

Conjecture 1.1 [16]**.** If $n \geq 10$, then each pendent vertex of an n-vertex tree with minimal ABC index belongs to a pendent path of length k, $2 \leq k \leq 3$.

In what follows we will prove the conjecture.

2. Some properties of $(x+y-2)/xy$

Since $ABC(G)$ is just the sum of $\sqrt{[d(u)+d(v)-2]/[d(u)d(v)]}$ over all pairs of adjacent vertices u and v of G, it is purposeful to establish some properties of $\sqrt{\frac{x+y-2}{xy}}$.

For $x, y \geq 1$, let $f(x,y) = \sqrt{\frac{x+y-2}{xy}}$. Obviously, $f(x,y) = f(y,x)$.

Lemma 2.1 [15]**.** $f(x,1)$ strictly increases with x, $f(x,2) = \sqrt{\frac{1}{2}}$, and $f(x,y)$ strictly decreases with x for fixed $y \geq 3$.

Lemma 2.2. If $y \geq 3$, $f(x,y) > \sqrt{\frac{1}{x}}$.

Proof. $f(x,y) = \sqrt{\frac{x+y-2}{xy}} = \sqrt{\frac{1}{x} + \frac{y-2}{y}} > \sqrt{\frac{1}{x}}$. ∎

For $x \geq 2, y \geq 1$, let $g(x,y) = f(x,y) - f(x-1,y)$.

Lemma 2.3 [15]**.** $g(x,y) \leq g(x,2) < g(x,1)$ for $y \geq 2$, and for fixed y, $g(x,y)$ strictly decreases with x if $y = 1$, and increases with x for fixed $y \geq 2$.

Lemma 2.4 [10]**.** $g(x,y) \geq \sqrt{\frac{1}{x}} - \sqrt{\frac{1}{x-1}}$.

Lemma 2.5. For fixed $x \geq 2$, $g(x,y)$ strictly decreases with $y \geq 1$.

Proof. $g(x,y+1) - g(x,y) < 0$

$$\Leftrightarrow \sqrt{\frac{x+y-1}{x(y+1)}} - \sqrt{\frac{x+y-2}{(x-1)(y+1)}}] < \sqrt{\frac{x+y-2}{xy}} - \sqrt{\frac{x+y-3}{(x-1)y}}$$

$$\Leftrightarrow \sqrt{(x-1)y(x+y-1)} + \sqrt{x(y+1)(x+y-3)} < \sqrt{(x-1)(y+1)(x+y-2)} + \sqrt{xy(x+y-2)}$$

$$\Leftrightarrow (x-1)y(x+y-1) + x(y+1)(x+y-3) + 2\sqrt{x(x-1)y(y+1)(x+y-1)(x+y-3)}$$

$$< (x-1)(y+1)(x+y-2) + xy(x+y-2) + 2\sqrt{x(x-1)y(y+1)(x+y-2)^2}$$

$$\Leftrightarrow 2\sqrt{x(x-1)y(y+1)(x+y-1)(x+y-3)} < 2 + 2\sqrt{x(x-1)y(y+1)(x+y-2)^2}$$

$$\Leftarrow \sqrt{x(x-1)y(y+1)(x+y-1)(x+y-3)} \leq \sqrt{x(x-1)y(y+1)(x+y-2)^2}$$

$$\Leftrightarrow (x+y-1)(x+y-3) \leq (x+y-2)^2 .$$ ■

Corollary 2.6. For $x, y \geq 3$, $\sqrt{\frac{1}{x}} - \sqrt{\frac{1}{x-1}} \leq g(x,y) \leq \sqrt{\frac{x+1}{3x}} - \sqrt{\frac{x}{3(x-1)}}$.

Proof. From Lemmas 2.4 and 2.5, $\sqrt{\frac{1}{x}} - \sqrt{\frac{1}{x-1}} \leq g(x,y) \leq g(x,3) = \sqrt{\frac{x+1}{3x}} - \sqrt{\frac{x}{3(x-1)}}$. ■

3. Some structural features of trees with minimal *ABC* index

In this section, we investigate some structural features of the trees with minimal *ABC* index.

Lemma 3.1 [16]**.** If $n \geq 10$, then an n-vertex tree with minimal *ABC* index does not contain internal paths of length $k \geq 2$.

Corollary 3.2 [16]**.** Let T be an n-vertex tree with minimal *ABC* index, where $n \geq 10$. Then $[T]$ is a tree.

Lemma 3.3 [16]**.** If $n \geq 10$, then an n-vertex tree with minimal *ABC* index does not contain pendent paths of length $k \geq 4$.

Lemma 3.4 [16]**.** If $n \geq 10$, then an n-vertex tree with minimal *ABC* index contains at most one pendent path of length $k \geq 3$.

Lemma 3.5 [16]**.** If T is a tree with star-type pendent vertices and a pendent path of length ≥ 3, then there is either a tree T' without star-type pendent vertices, such that $ABC(T') < ABC(T)$ or there is a tree T'' without pendent paths of length ≥ 3, such that $ABC(T'') < ABC(T)$.

Lemma 3.6 [16]**.** If a tree T with minimal *ABC* index possesses a star-type pendent vertex attached to the vertex r, then pendent paths of length k, $2 \leq k \leq 3$, cannot exist on any vertex of T, whose degree is smaller than the degree of r.

4. Proving the conjecture

In order to prove Conjecture 1.1, we need two auxiliary results.

First, we introduce a result of Chen [17] considering the change of *ABC* index under a so-called "edge-shifting transformation". Let G be a non-trivial connected graph, and v a vertex of G. Let $G_{k,l}$ $(k \geq l \geq 1)$ denote the graph obtained from G by attaching on v a pendent path of length k and a pendent path of length l. Note that the degree of v in $G_{k,l}$ is ≥ 3.

Lemma 4.1 [17]**.** (1) If $k = l = 1$, then $ABC(G_{k,l}) > ABC(G_{k+1,l-1})$;

(2) If $l = 1$, $k \geq 2$, and $d(v) \geq 4$, then $ABC(G_{k,l}) > ABC(G_{k+1,l-1})$;

(3) If $l = 2$, $k \geq 2$, then $ABC(G_{k,l}) < ABC(G_{k+1,l-1})$;

(4) If $k \geq l \geq 3$, then $ABC(G_{k,l}) = ABC(G_{k+1,l-1})$.

For a connected graph G, the diameter of G, denoted by $diaG$, is the length of a longest path of G. If $n \geq 10$, T is an n-vertex tree with minimal ABC index, from Corollary 3.2 we know $[T]$ is a tree. Here we show that $dia[T] \geq 1$.

Lemma 4.2. If $n \geq 10$ and T is an n-vertex tree with minimal ABC index , then $dia[T] \geq 1$.

Proof. Suppose $dia[T] < 1$, i. e., $[T]$ is trivial or T is an n-vertex path. Construct another n-vertex tree T^* with $dia[T^*] = 1$ from an edge xy by attaching two pendent paths of length 2 on x, r pendent paths of length 2 on y, and s pendent path of length 3 on y, where $r = (n-6)/2$, $s = 0$ if n is even, and $r = (n-9)/2$, $s = 1$ if n is odd. Note that $d(y) \geq 3 = d(x)$ in T^*. From Lemma 2.1 it is easily seen that $ABC(T^*) < (n-1)\sqrt{\frac{1}{2}} \leq ABC(T)$, with the equality iff T possesses no pendent paths of length 1. ■

Now we are in the position to complete the proof of Conjecture 1.1.

Proof of Conjecture 1.1. Let T be an n-vertex tree with minimal ABC index, where $n \geq 10$. Equivalently, we will show that T possesses no pendent paths of length 1. By contradiction, suppose that T possesses $p \geq 1$ pendent paths of length 1. From Lemma 3.5, we assume that T possesses no pendent paths of length ≥ 3, i. e., each pendent path of T is of length 1 or 2. If there are 2 or more pendent paths of length 1 on a vertex of T, then from Lemma 4.1 (1) we can get another n-vertex tree with strictly smaller ABC index than $ABC(T)$. Hence assume that there is at most one pendent path of length 1 on a vertex of T. Moreover, from Lemma 4.2 we have $dia[T] \geq 1$, so $[T]$ has at least 2 leaves.

We first verify the following three claims.

Claim 1. Each of the p pendent paths of length 1 should be on a vertex of degree 3.

Suppose that there is (exactly) one pendent path of length 1 on a vertex of degree ≥ 4. Say xx_1 is a pendent path of length 1 on x with $d(x) \geq 4$. If x is a leaf of $[T]$, from Lemma 4.1

(2) we can get an n-vertex tree with strictly smaller ABC index than $ABC(T)$. Hence assume that x is a branching vertex of $[T]$. Let u be a leaf of $[T]$, and w the only neighbor of u in $[T]$ (w may be identical with x). Since there should be pendent paths of length 2 on u, from Lemma 3.6 we have $d(u) \geq d(x) \geq 4$. Then from Lemma 4.1 (2), each pendent paths on u is of length 2, so each neighbor of u other than w is of degree 2. Let uu_1u_2 be a pendent path of length 2 on u, and $T' = T - uu_1 + x_1u_1$. From Lemmas 2.1, 2.3 and 2.4

$$
\begin{aligned}
ABC(T) - ABC(T') &= [f(1,d(x)) + f(d(u),d(w))] - [\sqrt{\tfrac{1}{2}} + f(d(u)-1,d(w))] \\
&\geq \sqrt{\tfrac{3}{4}} - \sqrt{\tfrac{1}{2}} + g(d(u),d(w)) \\
&\geq \sqrt{\tfrac{3}{4}} - \sqrt{\tfrac{1}{2}} + g(4,d(w)) \\
&\geq \sqrt{\tfrac{3}{4}} - \sqrt{\tfrac{1}{2}} + \sqrt{\tfrac{1}{4}} - \sqrt{\tfrac{1}{3}} \\
&\approx 0.081568 > 0,
\end{aligned}
$$

so $ABC(T') < ABC(T)$, and Claim 1 is valid.

Claim 2. If T contains pendent paths of length 1 on a branching vertex of $[T]$, then there exists another n-vertex tree T'' with $ABC(T_1'') < ABC(T)$.

Suppose that x is a branching vertex of $[T]$ on which there is (exactly) one pendent path xx_1 of length 1. Then $d(x) = 3$ from Claim 1. Let u and z be the two neighbors of x in $[T]$.

Case 1. There is (exactly) one pendent path of length 1 on u.

From Claim 1 we have $d(u) = 3$. Let T'' be the tree constructed from T by deleting the two pendent paths of length 1 on x and u, identifying vertices x and u, and then attaching a pendent path of length 3 on $x\,(=u)$. Then

$$
\begin{aligned}
ABC(T) - ABC(T'') &= f(1,3) + f(1,3) + f(3,3) - 3\sqrt{\tfrac{1}{2}} \\
&= 2\sqrt{\tfrac{2}{3}} + \sqrt{\tfrac{4}{9}} - 3\sqrt{\tfrac{1}{2}} \\
&\approx 0.178339 > 0,
\end{aligned}
$$

so $ABC(T'') < ABC(T)$.

Case 2. There is no pendent path of length 1 on u.

Thus each vertex in $A = N(u) - \{x\}$ is of degree ≥ 2. Let T'' be the tree constructed from T by identifying vertices x and u, and then replacing xx_1 by a pendent path of length 2 on x. Note that in T'', the degree of $x\,(=u)$ is $d(u)+1\,(\geq 4)$. From Lemmas 2.1, 2.2 and 2.5

$$\begin{aligned}ABC(T)-ABC(T'') &= [f(1,3)+f(3,d(u))+f(3,d(z))+\textstyle\sum_{v\in A} f(d(u),d(v))]\\
&\quad -[2\sqrt{\tfrac{1}{2}}+f(d(u)+1,d(z))+\textstyle\sum_{v\in A} f(d(u)+1,d(v))]\\
&> \sqrt{\tfrac{2}{3}}+\sqrt{\tfrac{1}{3}}-2\sqrt{\tfrac{1}{2}}+[f(3,d(z))-f(d(u)+1,d(z))]\\
&\quad +\textstyle\sum_{v\in A}[f(d(u),d(v))-f(d(u)+1,d(v))]\\
&\geq \sqrt{\tfrac{2}{3}}+\sqrt{\tfrac{1}{3}}-2\sqrt{\tfrac{1}{2}}+[f(3,d(z))-f(d(u)+1,d(z))]\\
&\geq \sqrt{\tfrac{2}{3}}+\sqrt{\tfrac{1}{3}}-2\sqrt{\tfrac{1}{2}}+[f(3,d(z))-f(4,d(z))]\\
&\geq \sqrt{\tfrac{2}{3}}+\sqrt{\tfrac{1}{3}}-2\sqrt{\tfrac{1}{2}}-g(4,3)\\
&= \sqrt{\tfrac{2}{3}}+\sqrt{\tfrac{1}{3}}-2\sqrt{\tfrac{1}{2}}+\sqrt{\tfrac{4}{9}}-\sqrt{\tfrac{5}{12}}\\
&\approx 0.000803>0,\end{aligned}$$

so $ABC(T'')<ABC(T)$.

Hence Claim 2 is valid from Case 1 and 2.

Claim 3. $p\leq 1$.

From Claims 1 and 2, each of the p pendent paths of length 1 is on a leaf of $[T]$ of degree 3. Suppose uu_1 (xx_1) is the only pendent path of length 1 on u (x), where u and x are two different leaves of $[T]$ with $d(u)=d(x)=3$. Let z be the only neighbor of x in $[T]$, and let $T'''=T-xx_1+u_1x_1$. Then from Lemma 2.2,

$$\begin{aligned}ABC(T)-ABC(T''') &= f(1,3)+f(1,3)+f(3,d(z))-3\sqrt{\tfrac{1}{2}}\\
&\geq 2\sqrt{\tfrac{2}{3}}+\sqrt{\tfrac{1}{3}}-3\sqrt{\tfrac{1}{2}}\\
&\approx 0.089023>0,\end{aligned}$$

so $ABC(T''')<ABC(T)$, and Claim 3 is valid.

From Claims 1-3, T possesses exactly one pendent path uv of length 1, such that u is a leaf of $[T]$ with $d(u)=3$. Let x be a leaf of $[T]$ other than u. Let w (z) be the only neighbor of u (x) in $[T]$. Let uu_1u_2 be the only pendent path of length 2 on u, and xx_1x_2 a pendent path of length 2 on x.

We proceed to complete the proof by the following two cases.

Case 1. $d(x)=3$.

It is easily seen that $dia[T]\geq 2$, or $n=9<10$. Hence $w\neq x$ and $z\neq u$. Let $T_1=T-uu_1+xu_1$. From Lemmas 2.2 and 2.5 we have

$$ABC(T)-ABC(T_1)=[f(1,3)+f(3,d(w))+f(3,d(z))]-[2\sqrt{\tfrac{1}{2}}+f(4,d(z))]$$
$$\geq\sqrt{\tfrac{2}{3}}+\sqrt{\tfrac{1}{3}}-2\sqrt{\tfrac{1}{2}}-g(4,d(z))$$
$$\geq\sqrt{\tfrac{2}{3}}+\sqrt{\tfrac{1}{3}}-2\sqrt{\tfrac{1}{2}}-g(4,3)$$
$$=\sqrt{\tfrac{2}{3}}+\sqrt{\tfrac{1}{3}}-2\sqrt{\tfrac{1}{2}}+\sqrt{\tfrac{4}{9}}-\sqrt{\tfrac{5}{12}}$$
$$\approx 0.000803>0,$$

so $ABC(T_1)<ABC(T)$.

Case 2. $d(x)\geq 4$.

Note that each vertex in $N(x)-\{z\}$ is of degree 2. Let $T_2=T-xx_1+vx_1$. From Lemmas 2.3 and 2.4 we have

$$ABC(T)-ABC(T_2)=[f(1,3)+f(d(x),d(z))]-[\sqrt{\tfrac{1}{2}}+f(d(x)-1,d(z))]$$
$$=\sqrt{\tfrac{2}{3}}-\sqrt{\tfrac{1}{2}}+g(d(x),d(z))$$
$$\geq\sqrt{\tfrac{2}{3}}-\sqrt{\tfrac{1}{2}}+g(4,d(z))$$
$$\geq\sqrt{\tfrac{2}{3}}-\sqrt{\tfrac{1}{2}}+\sqrt{\tfrac{1}{4}}-\sqrt{\tfrac{1}{3}}$$
$$\approx 0.032040>0,$$

so $ABC(T_2)<ABC(T)$.

The proof of the conjecture is thus completed. ■

We end this section with the following theorem, summarizing some known structural features of trees with minimal *ABC* index.

Theorem 4.3. If $n\geq 10$ and T is an n-vertex tree with minimal *ABC* index, then

(1) T does not contain internal paths of length ≥ 2;

(2) each pendent path of T is of length 2 or 3, and T contains at most one pendent path of length 3.

(3) $[T]$ is a tree with $dia[T]\geq 1$.

5. Comments

In the present paper we show that trees with minimal *ABC* index cannot possess pendent paths of length 1. However, fully characterizing their structure remains an open problem. Hence it is necessary to find more structural features of them.

Let $n\geq 10$ and T be an n-vertex tree with minimal *ABC* index. In Lemma 4.2 we prove that $dia[T]\geq 1$. Actually, it is not hard to show that $dia[T]\geq 2$ if $n\geq 15$. Observing the n-

vertex trees with minimal *ABC* index ($15 \le n \le 30$) shown in Table 2 [16], we guess that $dia[T] = 2$.

Conjecture 5.1. If $n \ge 15$ and T is an n-vertex tree with minimal *ABC* index, then $dia[T] = 2$.

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