On Trees with Minimal Atom Bond Connectivity Index

M. B. Ahmadi, S. A. Hosseini, P. Salehi Nowbandegani

Department of Mathematics, College of Sciences, Shiraz University 71454, Shiraz, Iran
mbahmadi@shirazu.ac.ir, seyyed.saeed.hosseini@gmail.com, pouria.salehi@gmail.com

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Abstract
In a recent work, I. Gutman and B. Furtula posed the structure of trees with a single high-degree vertex and smallest ABC index [1]. Here we provide a family of trees with smaller ABC index in one case of their conjectures. The smallest tree violating the Gutman-Furtula conjecture has 312 vertices.

1. Introduction

Graph-based molecular structure descriptors (often referred to as “topological indices”) are useful tools for modeling physical and chemical properties of molecules, for design of pharmacologically active compounds, for recognizing environmentally hazardous materials, etc. [2–4]. The atom-bond connectivity index (ABC) is a molecular structure descriptor that recently found a remarkable application in rationalizing the stability of linear and branched alkanes as well as the strain energy of cycloalkanes [5,6]. Let G be a simple graph with vertex set \( V(G) \) and edge set \( E(G) \). The degree of a vertex \( v \) is denoted by \( d_v \). The atom bond connectivity index of \( G \) is defined as
The mathematical properties of this index were reported in [2,3,7-13].

I. Gutman and B. Furtula conjectured [1] that if \( n \equiv 4 \pmod{7} \), \( k \geq 6 \), and \( n = 7k + 11 \), then the minimum-ABC tree has the structure shown in Fig. 1. We denote such graphs with 7k+11 vertices by \( GF_k \).

In this case we found a family of graphs shown in Fig. 2, that have smaller ABC index than the above structures. We denote such graphs with 7k+11 vertices by \( AHS_k \).

\[
ABC(G) = \sum_{uv \in E(G)} \frac{d_u + d_v - 2}{d_u d_v}.
\]

It is easy to see that:

\[
ABC(GF_k) = k \sqrt[4]{\frac{k + 4}{4(k + 2)}} + 2 \sqrt[3]{\frac{k + 3}{3(k + 2)}} + \frac{6k + 8}{\sqrt{2}}
\]

and
Here we are going to show that $ABC(GF_k) > ABC(AHS_k)$ for $k \geq 43$.

If the inequality $ABC(GF_k) > ABC(AHS_k)$ holds, it implies that:

$$\frac{1}{2}\sqrt{k^3 + 4k^2} + \frac{1}{2\sqrt{3}}\sqrt{16k + 48} > \frac{1}{2}\sqrt{k^3 + 6k^2 + 11k + 6} + \frac{1}{2\sqrt{3}}\sqrt{5k + 10}$$

By elementary calculation and squaring the above relation and rearranging for three times, we get

$$4k^8 - 120k^7 - 1900k^6 - \frac{26960}{4}k^5 - \frac{146480}{9}k^4 - \frac{46400}{9}k^3 + 14720k^2 + \frac{102400}{9}k + 6400 > 0$$

The largest root of the above polynomial is 42.480136, and its degree is even, therefore the value of the above polynomial is positive for $k > 42.480136$. Thus we have

$$ABC(GF_k) > ABC(AHS_k) \quad \text{for} \quad k \geq 43,$$

and the proof is complete.

One can ask about the behavior of $ABC(GF_k)$ and $ABC(AHS_k)$ for sufficiently large $k$. To answer this question we show that

$$\lim_{k \to \infty} ABC(GF_k) - ABC(AHS_k) = 0.0092.$$
Below we present numerical result showing that
\[
\frac{-2k^2 - 11k - 6}{4(k + 2)} + \frac{2}{\sqrt{3}} - \sqrt{\frac{5}{12}}
\]
for \( k \geq 43 \). Let \( A = ABC(GF_k) - ABC(AHS_k) \).

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### Table 1. ABC index for trees \( GF_k \) and \( AHS_k \), \( k = 6, \ldots, 80 \).

We conclude this section with a related conjecture about this problem. Let \( T \) be a tree with \( n \) vertices with a single high-degree vertex denoted by \( GF \), which is introduced in [1]. Then \( ABC(T) \) and \( ABC(GF) \) have the same behavior for sufficiently large \( n \), i. e.,

\[
\lim_{n \to \infty} ABC(GF) - ABC(T) \leq c
\]

where \( c \) is a sufficiently small constant.
References


