Applied Mathematics and Computation 282 (2016) 276–290

Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

On structural properties of trees with minimal atom-bond connectivity index III: Trees with pendent paths of length three☆

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ARTICLE INFO

Keywords:
Atom-bond connectivity index
Topological indices
Extremal graphs
Chemical applications

ABSTRACT

The *atom-bond connectivity (ABC) index* is a degree-based graph topological index that found chemical applications, including those of predicting the stability of alkanes and the strain energy of cycloalkanes. Several structural properties of the trees with minimal *ABC* index were proved recently, however the complete characterization of the minimal-ABC trees is still an open problem. It is known that minimal-ABC trees can have at most one pendent path of length 3. It is also known that the minimal-ABC trees that have a pendent path of length 3 do not contain so-called B_k-branches, with $k \geq 4$, and do not contain more than two B_2-branches. Here, we improve the latter result by showing that minimal-ABC trees of order larger than 168 and with a pendent path of length 3 do not contain B_2-branches. Moreover, we show that trees with minimal ABC index with a pendent path of length 3 do not contain B_1-branches.

1. Introduction

The *atom-bond connectivity (ABC) index* is a molecular-graph based structure descriptor, introduced in 1998 by Estrada et al. [18], who showed that it can be a valuable predictive tool in the study of the heat of formation in alkenes. Initially, it attracted little attention in mathematical chemistry, but after the publication of Estrada's second paper on this topic [17], where a novel quantum-theory-like justification for this topological index was elaborated, the interest of ABC-index has grown rapidly. Since then, the ABC index has attracted a lot of interest both in mathematical and chemical research communities, and numerous results, structural properties and variants of ABC index were established [1–7,9–11,14,19–21,23–25,28,30,32,37,39–42,44–46]. Additionally to [17], the physico-chemical applicability of the ABC index was confirmed and extended in several studies [8,12,26,31,34,47]. For other interesting degree-based indices, such as Zagreb index or Randić index the reader is referred to [27,35], respectively.

Let $G = (V, E)$ be a simple undirected graph of order $n = |V|$ and size $m = |E|$. For $v \in V$, the degree of v, denoted by $d(v)$, is the number of edges incident to v. For an edge uv in G, let

$$f(d(u), d(v)) = \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}}. \tag{1}$$

☆ This work was supported and funded by Kuwait University Research Grant no. SM06/15.
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http://dx.doi.org/10.1016/j.amc.2016.02.019
0096-3003/

Then, the atom-bond connectivity (ABC) index of G is defined as

$$\mathrm{ABC}(G) = \sum_{uv \in E} f(d(u), d(v)).$$

In [10] it was shown that adding an edge in a graph strictly increases its ABC index. Equivalently, in [5] it was shown that deleting an edge in a graph strictly decreases its ABC index. This revelation has the following two immediate consequences. Firstly, one can conclude that among all connected graphs with n vertices, the complete graph K_n has maximal value of ABC index. Secondly, it follows that among all connected graphs with n vertices, the graph with minimal ABC index is a tree.

In [21] it was proven that the star graph S_n is the tree with maximal ABC index. Although recently there was a significant progress in the characterization of the trees with minimal ABC index (also refereed as minimal-ABC trees), the full characterization is not yet completed. The aim of this work is to make a step forward towards the full characterizations of minimal-ABC trees.

Next, we present an additional notation that will be used in the rest of the paper. A tree is called a *rooted tree* if one vertex has been designated the *root*. In a rooted tree, the *parent* of a vertex is the vertex adjacent to it on the path to the root; every vertex except the root has a unique parent. A vertex is a parent of a subtree, if the subtree is attached to the vertex. A *child* of a vertex v is a vertex of which v is the parent. A vertex of degree one is a *pendent vertex*.

For the next two definitions, we adopt the notation from [30]. Let $u_0 u_1 \ldots u_{k-1} u_k$, $1 \le k \le n-1$, be a sequence of vertices of a graph G with $d(u_0) > 2$ and $d(u_i) = 2$, $i = 1, \ldots, k-1$. If $d(u_k) = 1$, then $u_0 \ldots u_{k-1} u_k$ is a *pendent path* of length k. If $d(u_k) > 2$, then $u_0 \ldots u_{k-1} u_k$ is an *internal path* of length k.

In Section 2 preliminaries and some known structural properties of the minimal-ABC trees, relevant to the work here, are given. In Section 3 minimal-ABC trees with pendent path of length 3 are considered. There, we improve the results from [16] by showing that minimal-ABC trees of order larger than 168 and with a pendent path of length 3 do not contain B_2-branches. In addition, we show that trees with minimal ABC index with a pendent path of length 3 do not contain B_1-branches. In the Appendix we present some technical results that are used in the proofs in Section 3.

2. Preliminaries and related results

An overview of most of the known structural properties of the minimal-ABC trees one can find in [14,29]. In this section, we present only the known properties that are relevant to this work. Results obtained by computer supported search can be found in [13,22,36,38]. Since, to determine the minimal-ABC trees of order less than 10 is an easy task, to simplify the exposition in the rest of the paper, we assume that the trees of interest are of order at least 10.

In [30], Gutman et al. obtained the following results.

Theorem 2.1. *The n-vertex tree with minimal ABC index does not contain internal paths of any length* $k \ge 2$.

Theorem 2.2. *The n-vertex tree with minimal ABC index does not contain pendent paths of length* $k \ge 4$.

An immediate, but important, consequence of Theorem 2.1 is the next corollary.

Corollary 2.3. *Let T be a tree with minimal ABC index. Then the subgraph induced by the vertices of T whose degrees are greater than two is also a tree.*

An improvement of Theorem 2.2 is the following result by Lin et al. [37].

Theorem 2.4. *Each pendent vertex of an n-vertex tree with minimal ABC index belongs to a pendent path of length k*, $2 \le k \le 3$.

Theorem 2.5 [30]**.** *The n-vertex tree with minimal ABC index contains at most one pendent path of length 3.*

Before we state the next important result, we consider the following definition of a *greedy tree* provided by Wang in [43].

Definition 2.1. Suppose the degrees of the non-leaf vertices are given, the greedy tree is achieved by the following 'greedy algorithm':

1. Label the vertex with the largest degree as v (the root).
2. Label the neighbors of v as $v_1, v_2, \ldots,$ assign the largest degree available to them such that $d(v_1) \ge d(v_2) \ge \cdots$
3. Label the neighbors of v_1 (except v) as $v_{11}, v_{12}, \ldots$ such that they take all the largest degrees available and that $d(v_{11}) \ge d(v_{12}) \ge \cdots$ then do the same for $v_2, v_3, \ldots$.
4. Repeat 3. for all newly labeled vertices, always starting with the neighbors of the labeled vertex with largest whose neighbors are not labeled yet.

Trees with minimal ABC index with prescribed degree sequences are characterized by the following result by Gan et al. [24]. Using slightly different notation and approach, the same result was obtained by Xing and Zhou [44].

Theorem 2.6. *Given the degree sequence, the greedy tree minimizes the ABC index.*