Discrete Applied Mathematics ▮ (▮▮▮▮) ▮▮▮–▮▮▮

Contents lists available at ScienceDirect

Discrete Applied Mathematics

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

On structural properties of trees with minimal atom-bond connectivity index II: Bounds on B_1- and B_2-branches

Darko Dimitrov

Hochschule für Technik und Wirtschaft Berlin, Wilhelminenhofstraß e 75A, D-12459 Berlin, Germany

ARTICLE INFO

Article history:
Received 22 December 2014
Received in revised form 9 October 2015
Accepted 13 October 2015
Available online xxxx

Keywords:
Atom-bond connectivity index
Topological indices
Extremal graphs

ABSTRACT

The *atom-bond connectivity (ABC) index* is a degree-based topological index that found chemical applications. The problem of complete characterization of trees with minimal *ABC* index is still an open problem. In an earlier paper, it was shown that trees with minimal ABC index do not contain so-called B_k*-branches*, with $k \geq 5$, and that they do not have more than four B_4-branches. Our main results here reveal that the number of B_1 and B_2-branches are also bounded from above by small fixed constants. Namely, we show that trees with minimal ABC index do not contain more than four B_1-branches and more than eleven B_2-branches.

1. Introduction

Let $G = (V, E)$ be a simple undirected graph of order $n = |V|$ and size $m = |E|$. For $v \in V(G)$, the degree of v, denoted by $d(v)$, is the number of edges incident to v. The *atom-bond connectivity (ABC) index* of G is defined as

$$\mathrm{ABC}(G) = \sum_{uv \in E(G)} \sqrt{\frac{(d(u) + d(v) - 2)}{d(u)d(v)}}.$$

The ABC index was introduced in 1998 by Estrada, Torres, Rodríguez and Gutman [16], who showed that it can be a valuable predictive tool in the study of the heat of formation in alikeness. Ten years later Estrada [15] elaborated a novel quantum-theory-like justification for this topological index. After that revelation, the interest of ABC-index has grown rapidly. Additionally, the physico-chemical applicability of the ABC index was confirmed and extended in several studies [4,8,12,22,26,29,38].

As a new and well motivated graph invariant, the ABC index has attracted a lot of interest in the last several years both in mathematical and chemical research communities and numerous results and structural properties of ABC index were established [5–7,9,14,10,11,17,18,20,21,23,25,27,31–33,35–37].

The fact that adding an edge in a graph strictly increases its ABC index [10] (or equivalently that deleting an edge in a graph strictly decreases its ABC index [5]) has the following two immediate consequences.

Corollary 1.1. *Among all connected graphs with n vertices, the complete graph K_n has maximal value of ABC index.*

Corollary 1.2. *Among all connected graphs with n vertices, the graph with minimal ABC index is a tree.*

E-mail address: darko.dimitrov11@gmail.com.

http://dx.doi.org/10.1016/j.dam.2015.10.010

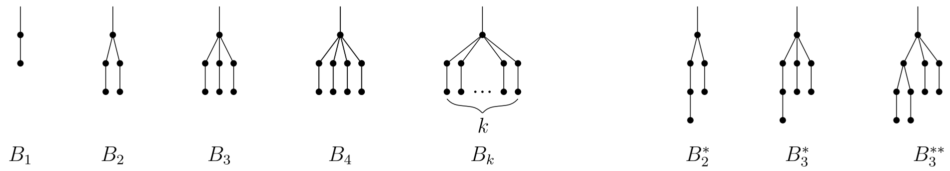

Fig. 1. B_k-branches.

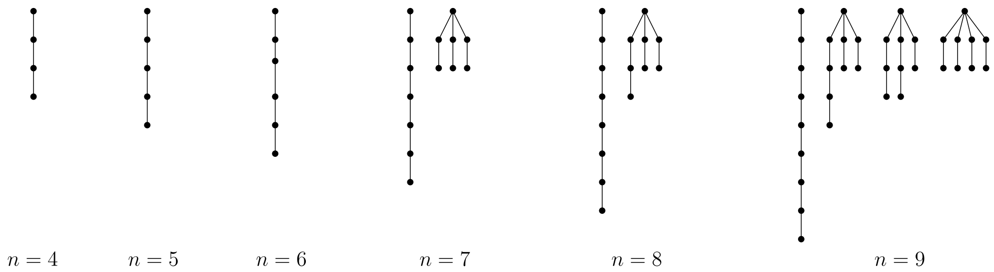

Fig. 2. Minimal-ABC trees of order n, $4 \leq n \leq 9$.

Although it is fairly easy to show that the star graph S_n is a tree with maximal ABC index [18], despite many attempts in the last years, it is still an open problem the characterization of trees with minimal ABC index (also refereed as minimal-ABC trees). The aim of this research is to make a step forward towards the full characterizations of minimal-ABC trees.

In the sequel, 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 connected 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 *pendant vertex*.

For the next two definitions, we adopt the notation from [24]. Let $S_k = v_0 \, v_1 \dots v_k, v_{k+1}$, $k \leq n - 3$, be a sequence of vertices of a graph G with $d(v_0) > 2$ and $d(v_i) = 2$, $i = 1, \dots k - 1$. If $d(v_k) = 1$, then S_k is a *pendant path* of length $k + 1$. If $d(v_k) > 2$, then S_k is an *internal path* of length k.

The so-called B_k-branches, subgraphs that are considered in the minimal-ABC trees, are illustrated in Fig. 1.

In Section 2 we give an overview of already known structural properties of the minimal-ABC trees. In Sections 3 and 4 we present some results and bounds on the number of B_1 and B_2-branches, respectively, that may occur in minimal-ABC trees. Conclusion and open problems are presented in Section 5.

2. Preliminaries and known structural properties of the minimal-ABC trees

A thorough overview of the known structural properties of the minimal-ABC trees was given in [24]. In addition to the results mentioned there, we present here also the recently obtained related results that we are aware of.

To determine the minimal-ABC tress of order less than 10 is a trivial task, and those trees are depicted in Fig. 2. To simplify the exposition in the rest of the paper, we assume that the trees of interest are of order at least 10.

In [25], Gutman, Furtula and Ivanović obtained the following results.

Theorem 2.1. *The n-vertex tree with minimal ABC-index does not contain internal paths of any length* $k \geq 1$.

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

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, Lin, Gao and Wu [31].

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

Theorem 2.5 ([25]). *The n-vertex tree with minimal ABC-index contains at most one pendant path of length 3.*

Before we state the next important result, we consider the following definition of a *greedy tree* provided by Wang in [34].

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

Please cite this article in press as: D. Dimitrov, On structural properties of trees with minimal atom-bond connectivity index II: Bounds on B_1- and B_2-branches, Discrete Applied Mathematics (2015), http://dx.doi.org/10.1016/j.dam.2015.10.010