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On structural properties of trees with minimal atom-bond connectivity index

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ABSTRACT

The *atom-bond connectivity (ABC) index* is a degree-based topological index, that found chemical applications. It is well known that among all connected graphs, the graphs with minimal ABC index are trees. A complete characterization of trees with minimal ABC index is still an open problem. In this paper, we present new structural properties of trees with minimal ABC index. Our main results reveal 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.

1. Introduction

Description of the structure or shape of molecules is very helpful in predicting activity and properties of molecules in complex experiments. For that purpose, the molecular descriptors [41] as mathematical quantities are particularly useful. Among the molecular descriptors, so-called topological indices [17] play a significant role. The topological indices can be classified by the structural properties of graphs used for their calculation. For example, the Wiener index [44] and the Balaban J index [4] are based on the distance of vertices in the respective graph, the Estrada index [19] and the energy of a graph [29] are based on the spectrum of the graph, the Hosoya index [36] is calculated by the counting of non-incident edges in a graph, while the Zagreb group indices [35] and the Randić connectivity index [40] depend on the degrees of vertices (for more details about degree-based topological indices, see the recent review paper [30]). On the other hand, there is a group of so-called information indices that are based on information functionals [5]. More about the information indices and the discriminative power of some established indices, one can find in [14–16,24] and in the works cited therein.

Here, we consider a relatively new topological index which attracted a lot of attention in the last few years. Namely, in 1998, Estrada et al. [21] proposed a new vertex-degree-based graph topological index, the *atom-bond connectivity (ABC) index*, and showed that it can be a valuable predictive tool in the study of the heat of formation in alkanes. Ten years later Estrada [20] elaborated a novel quantum-theory-like justification for this topological index. After that revelation, the interest in ABC-index has grown rapidly. Additionally, the physico-chemical applicability of the ABC index was confirmed and extended in several studies [3,9,13,28,34,38,48].

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. For an edge uv in G, let

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

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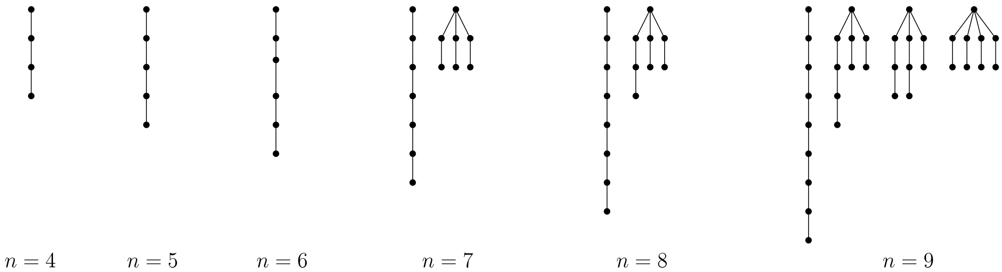

Fig. 1. Minimal-ABC trees of order n, $4 \le n \le 9$.

Then the atom-bond connectivity index of G is defined as

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

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 [6–8,10–12,22,23,31,33,26,39,42,45–47].

The fact that adding an edge in a graph strictly increases its ABC index [11] (or equivalently that deleting an edge in a graph strictly decreases its ABC index [6]) 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.*

Although it is fairly easy to show that the star graph S_n is a tree with maximal ABC index [23], 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 Section 2 we give an overview of already known structural properties of the minimal-ABC trees, while in Section 3 we present a few new properties. In the appendix we present some simpler results that are used in the proofs in Section 3.

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 *child* of a vertex v is a vertex of which v is the parent. A vertex of degree one is a *pendant vertex*. The *breadth-first search* is a graph search algorithm that begins at the root vertex and explores all its children vertices, beginning with the most right child and ending with the most left child. Then for each of those children, it explores their unexplored children vertices, and so on, until it finds the goal, or until all vertices are explored.

For the next two definitions, we adopt the notation from [32]. Let $S_k = v_0 v_1 \cdots v_k$, $k \le n-3$, be a sequence of vertices of a graph G with $d(v_0) > 2$ and $d(v_i) = 2$, $i = 1, \ldots, k-1$. If $d(v_k) = 1$, then S_k is a *pendant path* of length k. If $d(v_k) > 2$, then S_k is an *internal path* of length $k-1$.

2. Known structural properties of the minimal-ABC trees and some related results

A thorough overview of the known structural properties of the minimal-ABC trees was given in [32]. In addition to the results mentioned there, we also present here 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. 1. To simplify the exposition in the rest of the paper, we assume that the trees of interest are of order at least 10.

In [33], Gutman, Furtula and Ivanović obtained the following results.

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

Theorem 2.2. *An n-vertex tree with minimal ABC index does not contain pendant 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 and Gao [39].

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