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On a family of trees with minimal atom-bond connectivity index

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ABSTRACT

Let $G = (V, E)$ be a graph, d_i the degree of the vertex i, and ij the edge incident to the vertices i and j. The atom-bond connectivity index (or, simply, ABC index) is defined as $ABC(G) = \sum_{ij\in E} \sqrt{(d_i + d_j - 2)/(d_i d_j)}$. While this vertex-degree-based graph invariant is relatively well-known in chemistry, only recently a significant number of results emerged among the mathematical community. Though, several important problems remained open. One of them is the characterization of the tree(s) with minimal ABC index. In this paper, we will present some structural properties of one family of trees containing a pendent path of length 3 which would minimize the ABC index, mainly including: it contains no the so-called B_k with $k \geqslant 4$, and contains at most two B_2's.

1. Introductions and preliminaries

Let $G = (V, E)$ be a graph, d_i the degree of the vertex i, and ij the edge incident to the vertices i and j. The atom-bond connectivity index (or, simply, ABC index) is a vertex-degree-based graph topological index defined as

$$ABC(G) = \sum_{ij\in E} \sqrt{\frac{d_i + d_j - 2}{d_i d_j}},$$

and it can be seen as a modification of the Randić graph-theoretic invariant [17].

The importance of the ABC index was first revealed in 1998. In fact, it was showed in [6] that the ABC index can be a helpful analytical instrument for modeling thermodynamic properties of organic chemical compounds.

A decade later, Estrada [5] based on a novel quantum-theory-like elucidation, exposed again the importance of this index on the stability of branched alkanes. Since then, a large number of mathematical directly related papers have emerged. According to Gutman [9], the ABC index *happens to be the only topological index for which a theoretical, quantum-theory-based, foundation and justification have been found*.

As in many mathematical problems, characterizing the graph(s) and, in particular, the tree(s) with extremal values of an index is of crucial importance. While the study of the tree(s) with maximal ABC index has been completely determined – the star – in [7], for the tree(s) with minimal ABC index, some interesting questions remain open. Several conjectures (and sometimes surprising disproofs) are known, as well as some partial results have recently been found (see, e.g., [1,2,4,10,11,15,16]).

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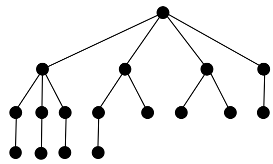

Fig. 1.1. An example of greedy tree.

For example, the catacondensed hexagonal systems with extremal ABC indices were characterized in [15] and it was shown that the ABC index of a graph decreases when any edge is deleted. In [14] the so-called breadth-first searching graphs were introduced in order to obtain the minimal value or lower bounds of ABC index of connected graphs. More recently, trees with minimal ABC index among the so-called Kragujevac trees were determined in [13].

A path $v_0v_1\dots v_r$ in a graph G is said to be a pendent path of length r, where $d_{v_0} \geqslant 3$, $d_{v_1} = \cdots = d_{v_{r-1}} = 2$, and $d_{v_r} = 1$.

For the tree(s) with minimal ABC index, the lengths of its pendent paths are of crucial importance. In particular, the next lemma has become a key result in this area:

Lemma 1.1 ([12,15]). *If T is a tree with minimal ABC index, then every pendent path in T is of length 2 or 3, and there is at most one pendent path of length 3 in T.*

Recently, Dimitrov [3] presented a new approach for computing trees with minimal ABC index. By considering the degree sequences of trees and some known properties of the trees with minimal ABC index, and together with some existing counterexamples, Dimitrov set some new conjectures. One of them is the following:

Conjecture 1 ([3]). *If T is a tree of order $n > 1178$ with minimal ABC index, then there is no pendent path of length 3 in T.*

Before we proceed, let us recall that, according to Wang [18], for a given degree sequence of the vertices of degree more than 1, the greedy tree T is a rooted tree achieved by

(i) Label the vertex with the largest degree as i;
(ii) Label the neighbors of i as $i_1, i_2, \dots$; assign the largest degree available to them such that $d_{i_1} \geqslant d_{i_2} \geqslant \cdots$;
(iii) Label the neighbors of i_1 (except i) as $i_{11}, i_{12}, \dots$, such that they take all the largest degrees available and $d_{i_{11}} \geqslant d_{i_{12}} \geqslant \cdots$;
(iv) Repeat (iii) for all the newly labeled vertices, always start with the neighbors of the labeled vertex with largest degree whose neighbors are not labeled yet.

In particular, the vertex i is said to be the root of T, which is also the vertex lying on the first layer of T; the vertices $i_1, i_2, \dots$ are said to be the vertices lying on the second layer of T; the vertices $i_{11}, i_{12}, \dots$ are said to be the vertices lying on the third layer of T, and so on.

For example, the tree as shown in Fig. 1.1 is a greedy tree with degree sequence

$$(4, 4, 3, 3, 2, 2, 2, 2, 2).$$

In particular, the first vertex of degree 4 is the root of the tree.

Recently, it was pointed out that the minimal ABC index among trees would be attained by some greedy tree.

Lemma 1.2 ([8,19]). *Given the degree sequence, the greedy tree minimizes the ABC index.*

By Lemma 1.2, we know that if we want to consider trees with minimal ABC index, we need only to focus on the greedy trees.

In order to approach to a solution for Conjecture 1, in this paper we will reveal some structural properties of a greedy tree with minimal ABC index and containing a pendent path of length 3, mainly including: it contains no the so-called B_k with $k \geqslant 4$, and contains at most two B_2's.

2. Graph transformations

In this section, we will introduce some graph transformations and consider the effect on ABC index under such transformations.

The following lemma is clear and, therefore, we state it without a proof.

Lemma 2.1 ([13]). *Let T be a tree. Suppose that $v_1v_2v_3$ is a pendent path of length 2 in T, and $wu_1u_2u_3$ is a pendent path of length 3 in T, where v_1 and w are the pendent vertices of T. Let T_1 be the tree obtained from T by deleting the edge wu_1 and adding the edge wv_1. Then $ABC(T) = ABC(T_1)$.*

Let B_1, B_1^*, B_k with $k \geqslant 2$, and B_k^* with $k \geqslant 2$ be, respectively, the branches of trees defined as shown in Fig. 2.1. For convenience, a branch B_k with $k \geqslant 1$ is said to be a B_k-type branch, and a branch B_k^* with $k \geqslant 1$ is said to be a B_k^*-type branch.