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Note

The maximum atom-bond connectivity index for graphs with edge-connectivity one

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ABSTRACT

The atom-bond connectivity (ABC) index of a graph G is defined as the sum of the weights $\sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}$ of all edges uv of G, where $d(u)$ denotes the degree of a vertex u in G. In this short note, we determine the maximum ABC index for graphs with edge-connectivity one and characterize the corresponding extremal graphs. This answers a recent question proposed by Zhang et al. (2016).

1. Introduction

Molecular descriptors are playing a significant role in chemistry, pharmacology, etc. Among them, topological indices have a prominent place. Topological indices are numbers associated with chemical structures derived from their hydrogen-depleted graphs as a tool for compact and effective description of structural formulas which are used to study and predict the structure–property correlations of organic compounds. There are lots of topological indices which have found some applications in theoretical chemistry, especially in QSPR/QSAR studies (for example, see [20, pages 34–95] and [21, pages 105–140]).

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. The atom-bond connectivity (ABC) index was introduced by Estrada et al. [13] in 1998. This index is defined as

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

where $d(u)$ denotes the degree of a vertex u of G. It displays an excellent correlation with the heat of formation of alkanes [13], and a basically topological approach was developed on the basis of the ABC index to explain the differences in the energy of linear and branched alkanes both qualitatively and quantitatively [12].

The mathematical properties of the ABC index have been studied extensively. Furtula, Graovac and Vukičević [14] determined the maximum ABC index for trees and the maximum and minimum ABC indices for chemical trees. Xing, Zhou and Du [23] found the maximum ABC indices for trees with a perfect matching or given maximum degree, and characterized the corresponding extremal trees. See [1–11,15–19,22,25] for more information of this index.

Recently, Zhang et al. [24] considered the maximum ABC indices for connected graphs with some given graph parameters such as independence number, number of pendent vertices, edge-connectivity and chromatic number. Particularly, they

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Table 1
The ABC indices of K_n^* and all possible graphs G^* (for $6 \leq n \leq 12$).

n	n_1	n_2	$ABC(G^*)$	$ABC(K_n^*)$	n	n_1	n_2	$ABC(G^*)$	$ABC(K_n^*)$
6	3	3	4.9093	6.9350		3	8	16.4987	
7	3	4	6.7033	9.3083	11	4	7	15.4797	20.8602
8	3	5	8.7944	11.9021		5	6	14.9839	
	4	4	8.4854			3	9	19.4772	
9	3	6	11.1404	14.7004	12	4	8	18.2605	24.2014
	4	5	10.5688			5	7	17.5515	
	3	7	13.7148			6	6	17.3180	
10	4	6	12.9093	17.6901					
	5	5	12.6470						

determined the maximum ABC index for graphs with edge-connectivity k ($k \geq 2$) and characterized the corresponding extremal graphs. It was suggested in [24] that the extremal graphs with the maximum ABC index for graphs with edge-connectivity 1 might have the similar structure as in the general case (i.e., $k \geq 2$). In this short note, we give an affirmative answer to this question.

2. Main result

In this section, we prove the main result of this paper. First, we list the following two lemmas which will be used in our proof. The first lemma was proved by Chen and Guo [2] (see also [4]).

Lemma 2.1. *Let G be a graph with n vertices. If x and y are two nonadjacent vertices in G, then $ABC(G) \leq ABC(G + xy)$ with equality if and only if both x and y are isolated vertices of G. As a consequence, we have $ABC(G) \leq ABC(K_n)$ with equality if and only if $G \cong K_n$, where K_n denotes the complete graph with n vertices.*

The second lemma was shown in [23,22].

Lemma 2.2. *Let $f(x, y) = \sqrt{\frac{x+y-2}{xy}}$ with $x, y \geq 1$, then $f(x, y)$ is decreasing with respect to x for any fixed $y \geq 2$.*

For $n \geq 3$, let K_n^* be the graph on n vertices obtained by attaching a pendent vertex to exactly one vertex of K_{n-1}. It is easy to see that K_n^* has edge-connectivity 1. We now prove the main result of this paper by applying the similar idea as in [24].

Theorem 2.3. *Let G be a graph with $n \geq 3$ vertices and edge-connectivity 1. Then*

$$ABC(G) \leq \sqrt{\frac{n-2}{n-1}} + \frac{n-3}{2}\sqrt{2n-6} + (n-2)\sqrt{\frac{2n-5}{(n-1)(n-2)}}$$

with equality if and only if $G \cong K_n^*$.

Proof. Suppose G^* is the graph with the maximum ABC index among all graphs with $n \geq 3$ vertices and edge-connectivity 1.

First, suppose G^* contains a vertex of degree 1, say v. Let $G' := G^* - \{v\}$. Then by Lemma 2.1 and by the assumption of G^*, we see that G' is the complete graph on $n-1$ vertices; for otherwise, there must exist two nonadjacent vertices x, y in G' such that the graph $G^* + \{xy\}$ has edge-connectivity 1 and $ABC(G^* + \{xy\}) > ABC(G^*)$, a contradiction. This implies that $G^* \cong K_n^*$, and hence the assertion holds.

So we may assume that every vertex in G^* has degree at least 2. Let e be a cut-edge in G^*. Then $G^* - \{e\}$ has exactly two components, say G_1 and G_2. By Lemma 2.1 and by the assumption of G^*, we have both G_1 and G_2 as complete graphs. Let n_i be the number of vertices in G_i (for $i = 1, 2$), then $n = n_1 + n_2$. Without loss of generality, we may assume $n_2 \geq n_1$. Since G^* has minimum degree at least 2, we have $n_2 \geq n_1 \geq 3$ and hence $n \geq 6$.

For each $6 \leq n \leq 12$, there are only a few possible graphs satisfying the conditions that both components G_1 and G_2 are complete graphs and $n_2 \geq n_1 \geq 3$. So it is easy to check that the assertion holds for $6 \leq n \leq 12$ through direct calculations (see Table 1). Therefore we may further assume that $n \geq 13$.

Since $n_2 \geq n_1 \geq 3$ (and $n \geq 13$), by Lemma 2.2, we have

$$\begin{aligned}
ABC(K_n^*) &= f(1, n-1) + (n-2)f(n-1, n-2) + \frac{(n-2)(n-3)}{2}f(n-2, n-2) \\
&\geq f(1, n-1) + (n-2)f(n-1, n-1) + \frac{(n-2)(n-3)}{2}f(n-1, n-1) \\
&= f(1, n-1) + \frac{(n-1)(n-2)}{2}f(n-1, n-1) \\
&= \sqrt{\frac{n-2}{n-1}} + \frac{(n-2)^{\frac{3}{2}}}{\sqrt{2}}
\end{aligned}$$

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