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Extreme Atom-Bond Connectivity Index of Graphs *

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Abstract

The atom-bond connectivity (ABC) index of a graph G, is defined as the sum of the weights $\left(\frac{d_u+d_v-2}{d_u d_v}\right)^{\frac{1}{2}}$ of all edges uv of G, where d_u denotes the degree of a vertex u in G. The ABC index provides a good model for the stability of linear and branched alkanes as well as the strain energy of cycloalkanes. In this paper, we characterize the catacondensed hexagonal systems with extreme ABC indices, and prove that the ABC index of a graph decreases when any edge is deleted. Consequently, it is also proved that the graph with n vertices and the maximum ABC index is the complete graph K_n.

1 Introduction

A hexagonal system is a finite connected plane graph with no cut vertex in which every interior region is surrounded by a regular hexagon of side length 1. A hexagonal system

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without internal vertex is called catacondensed hexagonal system. Hexagonal systems are the natural graph representation of benzenoid hydrocarbons and have been widely investigated [3].

In the last few years a number of new molecular structure descriptors has been conceived (e.g., see [5,8-10]) and several of them have found applications in QSPR/QSAR studies. Among molecular structure descriptors, topological indices have a prominent place. One of the most important topological indices is the Randić index which is aimed at the modelling of the branching of the carbon-atom skeleton of alkanes, introduced by Randić [11]. But a great variety of physico-chemical properties lie on factors rather than branching. In order to take this into consideration, Estrada et al. proposed a new index, known as the atom-bond connectivity (ABC) index [6] of graph G, which is abbreviated as $ABC(G)$. $ABC(G)$ is defined as the sum of $\left(\frac{d_u+d_v-2}{d_u d_v}\right)^{\frac{1}{2}}$ over all edges uv of G, where d_u denote the degree of a vertex u of G, i.e.,

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u+d_v-2}{d_u d_v}}.$$

The ABC index keep the spirit of the Randić index, and it provides a good model for the stability of linear and branched alkanes as well as the strain energy of cycloalkanes [4,6].

Furtula et al. [7] studied the mathematical properties of ABC index of trees and proved that the star tree, S_n, has the maximal ABC value among all trees with $n(\geq 2)$ vertices. They also obtained the chemical trees with extremal ABC indices. In the present paper, we are interested in molecular structure with cycles, in particular, the catacondensed hexagonal systems. The catacondensed hexagonal systems with the maximum and minimum ABC indices among all catacondensed hexagonal systems with h hexagons are given.

Bollobás and Erdös [1] found that the Randić index of a graph decreases when an edge with maximal weight is deleted. For ABC index of graphs, we prove that the ABC index of a graph decreases when any edge is deleted. Consequently it is also proved that the graph with n vertices and the maximum ABC index is the complete graph K_n.

All graphs considered here are finite and simple. Undefined teminology and notation may refer to [2].

2 Extreme ABC index of catacondensed hexagonal systems

Let $\mathscr{C}_h$ be the set of catacondensed hexagonal systems with h hexagons. For a hexagonal system $C_h \in \mathscr{C}_h$, its dualist graph $D(C_h)$ is the graph whose vertex set is the set of hexagons of C_h, and two vertices of which are adjacent if the corresponding hexagons have a common edge. Clearly the dualist graph of a catacondensed hexagonal system is a tree with the maximum degree less than or equal to 3. For $C_h \in \mathscr{C}_h$, a hexagon s of C_h is called a kink of C_h if s has exactly two consecutive vertices of degree 2 in C_h, and called a branched hexagon if s has no vertex with degree 2 in C_h. A kink (resp. branched hexagon) of C_h corresponds to a vertex of degree 2 (resp. degree 3) in the dualist graph $D(C_h)$ of C_h. The catacondensed hexagonal systems having no kink and branched hexagon are called linear hexagonal chains. Let L_h be the linear hexagonal chain with h hexagons. Let $\mathscr{D}_h$ be the set of the catacondensed hexagonal systems with h hexagons for which the dualist graph of any hexagonal system $C_h \in \mathscr{D}_h$ has at most one vertex of degree 2, and the vertex of degree 2 corresponds to a kink of C_h. It is not difficult to see that any hexagonal system in $\mathscr{D}_h$ has exactly $\lfloor \frac{h-2}{2} \rfloor$ branched hexagons. Let $a(C_h)$ (resp. $b(C_h)$) be the number of kinks (resp. branched hexagons) in C_h.

In the following we can obtain the sharp lower and upper bounds on ABC index of catacondensed hexagonal systems.

Theorem 1. Let $C_h \in \mathscr{C}_h$, then

(i) $ABC(C_h) = (\sqrt{2} - \frac{2}{3}) + (\frac{2}{3} + 2\sqrt{2})h - (\frac{\sqrt{2}}{2} - \frac{2}{3})\Big(a(C_h) + 3b(C_h)\Big)$;

(ii) $ABC(C_h)$ is monotonously decreasing in $a(C_h)$ or $b(C_h)$;

(iii) $ABC(D_h) \leq ABC(C_h) \leq ABC(L_h)$, where L_h is the linear hexagonal chain with h hexagons and $D_h \in \mathscr{D}_h$.

Proof. (i) We prove (i) of Theorem 3 by induction on h.

If $h = 1$, then $a(C_1) = b(C_1) = 0$ and $ABC(C_1) = 3\sqrt{2}$, so (i) holds for $h = 1$.

If $h = 2$, then $a(C_2) = b(C_2) = 0$ and $ABC(C_2) = \frac{2}{3} + 5\sqrt{2}$, so (i) holds for $h = 2$.

If $h = 3$, then $b(C_3) = 0$. Suppose $a(C_3) = 0$ (resp. $a(C_3) = 1$), then $ABC(C_3) = \frac{4}{3} + 7\sqrt{2}$ (resp. $ABC(C_3) = 2 + \frac{13}{2}\sqrt{2}$), so (i) holds for $h = 3$.

Assume (i) holds for all $C_{h-1} \in \mathscr{C}_{h-1}$ ($h \geq 4$), i.e., $ABC(C_{h-1}) = (\sqrt{2} - \frac{2}{3}) + (\frac{2}{3} + 2\sqrt{2})(h-1) - (\frac{\sqrt{2}}{2} - \frac{2}{3})\Big(a(C_{h-1}) + 3b(C_{h-1})\Big)$. Let $C_h \in \mathscr{C}_h$, which is obtained by gluing a new hexagon s_h to some C_{h-1}. Without loss of generality, assume that the hexagon s_h is adjacent to some hexagon s_i in C_{h-1}. Now in C_h we have the following three cases.

Case 1. If s_i is a branched hexagon of C_h. Then $a(C_h) = a(C_{h-1}) - 1$ and $b(C_h) = b(C_{h-1}) + 1$. By the induction assumption and direct computation, we have

$$
\begin{aligned}
&ABC(C_h) = ABC(C_{h-1}) + (2 + \sqrt{2})\\
&= (\sqrt{2} - \frac{2}{3}) + (\frac{2}{3} + 2\sqrt{2})(h-1) - (\frac{\sqrt{2}}{2} - \frac{2}{3})\Big(a(C_{h-1}) + 3b(C_{h-1})\Big) + (2 + \sqrt{2})\\
&= (\sqrt{2} - \frac{2}{3}) + (\frac{2}{3} + 2\sqrt{2})h - (\frac{\sqrt{2}}{2} - \frac{2}{3})\bigg(\Big(a(C_{h-1}) - 1\Big) + 3\Big(b(C_{h-1}) + 1\Big)\bigg)\\
&= (\sqrt{2} - \frac{2}{3}) + (\frac{2}{3} + 2\sqrt{2})h - (\frac{\sqrt{2}}{2} - \frac{2}{3})\Big(a(C_h) + 3b(C_h)\Big).
\end{aligned}
$$

Case 2. If s_i is a kink of C_h. Then $a(C_h) = a(C_{h-1}) + 1$ and $b(C_h) = b(C_{h-1})$. By the induction assumption and direct computation, we have

$$
\begin{aligned}
&ABC(C_h) = ABC(C_{h-1}) + (\frac{4}{3} + \frac{3}{2}\sqrt{2})\\
&= (\sqrt{2} - \frac{2}{3}) + (\frac{2}{3} + 2\sqrt{2})(h-1) - (\frac{\sqrt{2}}{2} - \frac{2}{3})\Big(a(C_{h-1}) + 3b(C_{h-1})\Big) + (\frac{4}{3} + \frac{3}{2}\sqrt{2})\\
&= (\sqrt{2} - \frac{2}{3}) + (\frac{2}{3} + 2\sqrt{2})h - (\frac{\sqrt{2}}{2} - \frac{2}{3})\bigg(\Big(a(C_{h-1}) + 1\Big) + 3b(C_{h-1})\bigg)\\
&= (\sqrt{2} - \frac{2}{3}) + (\frac{2}{3} + 2\sqrt{2})h - (\frac{\sqrt{2}}{2} - \frac{2}{3})\Big(a(C_h) + 3b(C_h)\Big).
\end{aligned}
$$

Case 3. Otherwise, $a(C_h) = a(C_{h-1})$ and $b(C_h) = b(C_{h-1})$. By the induction assumption and direct computation, we have

$$ABC(C_h) = ABC(C_{h-1}) + (\frac{2}{3} + 2\sqrt{2})$$

$$= (\sqrt{2} - \frac{2}{3}) + (\frac{2}{3} + 2\sqrt{2})(h-1) - (\frac{\sqrt{2}}{2} - \frac{2}{3})\Big(a(C_{h-1}) + 3b(C_{h-1})\Big) + (\frac{2}{3} + 2\sqrt{2})$$
$$= (\sqrt{2} - \frac{2}{3}) + (\frac{2}{3} + 2\sqrt{2})h - (\frac{\sqrt{2}}{2} - \frac{2}{3})\Big(a(C_h) + 3b(C_h)\Big).$$

Therefore, (i) of Theorem 3 holds.

(ii) Obviously.

(iii) Since $0 = a(L_h) \le a(C_h)$, $0 = b(L_h) \le b(C_h)$, by (ii) we have $ABC(C_h) \le ABC(L_h)$.

Now, let us prove the lower bound. For any $D_h \in \mathscr{D}_h$, if h is even (resp. odd), then $a(D_h) = 0$ and $b(D_h) = \frac{h-2}{2}$ (resp. $a(D_h) = 1$ and $b(D_h) = \frac{h-3}{2}$). From (i), we have

$$ABC(D_h) = (\sqrt{2} - \frac{2}{3}) + (\frac{2}{3} + 2\sqrt{2})h - (\frac{\sqrt{2}}{2} - \frac{2}{3})\Big(a(D_h) + 3b(D_h)\Big)$$

$$= \begin{cases} (\sqrt{2} - \frac{2}{3}) + (\frac{2}{3} + 2\sqrt{2})h - (\frac{\sqrt{2}}{2} - \frac{2}{3}) \cdot \frac{3h-6}{2} & \text{(if } h \text{ is even)} \\ (\sqrt{2} - \frac{2}{3}) + (\frac{2}{3} + 2\sqrt{2})h - (\frac{\sqrt{2}}{2} - \frac{2}{3}) \cdot \frac{3h-7}{2} & \text{(if } h \text{ is odd)} \end{cases}$$
$$= (\sqrt{2} - \frac{2}{3}) + (\frac{2}{3} + 2\sqrt{2})h - (\frac{\sqrt{2}}{2} - \frac{2}{3})(h - 2 + \lfloor \frac{h-2}{2} \rfloor).$$

Since a kink (resp. branched hexagon) of C_h corresponds to a vertex of degree 2 (resp. degree 3) in the dualist graph $D(C_h)$ of C_h, and note that a vertex of degree 2 in $D(C_h)$ not necessarily corresponding to a kink of C_h, we have $2a(C_h)+3b(C_h)+\Big(h-a(C_h)-b(C_h)\Big) \le 2(h-1)$, i.e., $a(C_h)+2b(C_h) \le h-2$. It follows that $b(C_h) \le \lfloor \frac{h-2}{2} \rfloor$. From (i), we have

$$ABC(C_h) = (\sqrt{2} - \frac{2}{3}) + (\frac{2}{3} + 2\sqrt{2})h - (\frac{\sqrt{2}}{2} - \frac{2}{3})\Big(a(C_h) + 3b(C_h)\Big)$$
$$= (\sqrt{2} - \frac{2}{3}) + (\frac{2}{3} + 2\sqrt{2})h - (\frac{\sqrt{2}}{2} - \frac{2}{3})\left(\Big(a(C_h) + 2b(C_h)\Big) + b(C_h)\right)$$
$$\ge (\sqrt{2} - \frac{2}{3}) + (\frac{2}{3} + 2\sqrt{2})h - (\frac{\sqrt{2}}{2} - \frac{2}{3})(h - 2 + \lfloor \frac{h-2}{2} \rfloor).$$
$$= ABC(D_h).$$

□

3 The ABC index changes due to edge deletion

In this section, we will prove that the ABC index of a graph decreases when any edge is deleted. Consequently, it is proved that the graphs on n vertices with maximum ABC index is the complete graph K_n. We first give two lemmas.

Lemma 1. Let x_1x_2 be an edge of a graph G and let $d(x_i) = d_i$ $(i = 1, 2)$. If $d_1 = 1$, then $ABC(G - x_1x_2) \leq ABC(G)$, equality holds if and only if x_1x_2 is an isolate edge of G.

Proof. Let $E_0 = E(G) \setminus \{x_1x_2\}$. If $d_2 = 1$, then $ABC(G) - ABC(G - x_1x_2) = 0$; therefore we may assume that $d_2 \geq 2$.

Note that

$$\begin{aligned}
&ABC(G) - ABC(G - x_1x_2)\\
&= \frac{\sqrt{d_2-1}}{\sqrt{d_2}} + \sum_{x_2v\in E_0} \frac{\sqrt{d_2+d_v-2}}{\sqrt{d_2d_v}} - \sum_{x_2v\in E_0} \frac{\sqrt{(d_2-1)+d_v-2}}{\sqrt{(d_2-1)d_v}}\\
&= \frac{\sqrt{d_2-1}}{\sqrt{d_2}} + \sum_{x_2v\in E_0} \frac{\sqrt{d_2+d_v-2}}{\sqrt{d_2d_v}} - \sum_{x_2v\in E_0} \Big(\frac{\sqrt{d_2+d_v-2}}{\sqrt{d_2d_v}} \cdot \frac{\sqrt{d_2+d_v-3}}{\sqrt{d_2+d_v-2}} \cdot \frac{\sqrt{d_2}}{\sqrt{d_2-1}}\Big)\\
&> \frac{\sqrt{d_2-1}}{\sqrt{d_2}} + \sum_{x_2v\in E_0} \frac{\sqrt{d_2+d_v-2}}{\sqrt{d_2d_v}} - \sum_{x_2v\in E_0} \Big(\frac{\sqrt{d_2+d_v-2}}{\sqrt{d_2d_v}} \cdot \frac{\sqrt{d_2}}{\sqrt{d_2-1}}\Big)\\
&= \frac{\sqrt{d_2-1}}{\sqrt{d_2}} + \Big(1 - \frac{\sqrt{d_2}}{\sqrt{d_2-1}}\Big) \cdot \sum_{x_2v\in E_0} \frac{\sqrt{d_2+d_v-2}}{\sqrt{d_2d_v}}.
\end{aligned}$$

Since $\sum_{x_2v\in E_0} \frac{\sqrt{d_2+d_v-2}}{\sqrt{d_2d_v}} \leq (d_2-1) \cdot \frac{\sqrt{d_2-1}}{\sqrt{d_2}}$, we have

$$\begin{aligned}
&ABC(G) - ABC(G - x_1x_2)\\
&\geq \frac{\sqrt{d_2-1}}{\sqrt{d_2}} + \frac{(d_2-1)\sqrt{d_2-1}}{\sqrt{d_2}} \cdot \Big(1 - \frac{\sqrt{d_2}}{\sqrt{d_2-1}}\Big)\\
&= \frac{\sqrt{d_2-1}}{\sqrt{d_2}} + \frac{(d_2-1)\sqrt{d_2-1}}{\sqrt{d_2}} - (d_2-1)\\
&= \frac{\sqrt{d_2-1}}{\sqrt{d_2}} \cdot (d_2-1+1) - (d_2-1)\\
&= \sqrt{d_2(d_2-1)} - (d_2-1) > 0.
\end{aligned}$$

i.e., $ABC(G - x_1x_2) < ABC(G)$. □

Lemma 2. Let $x \in \{2\} \bigcup [3, +\infty)$, $y \in [1, +\infty)$, $f(x, y) = \dfrac{\sqrt{x+y-2}}{\sqrt{xy}} - \dfrac{\sqrt{x+y-3}}{\sqrt{(x-1)y}}$, then $f(x, y) \geq \dfrac{1}{\sqrt{x}} - \dfrac{1}{\sqrt{x-1}}$.

Proof. $\dfrac{\partial f}{\partial y} = \dfrac{\frac{\sqrt{xy}}{2\sqrt{x+y-2}} - \frac{x\sqrt{x+y-2}}{2\sqrt{xy}}}{xy} - \dfrac{\frac{\sqrt{(x-1)y}}{2\sqrt{x+y-3}} - \frac{(x-1)\sqrt{x+y-3}}{2\sqrt{(x-1)y}}}{(x-1)y}$
$= \dfrac{1}{2\sqrt{y^3}}\Big(\dfrac{x-3}{\sqrt{x-1} \cdot \sqrt{x+y-3}} - \dfrac{x-2}{\sqrt{x} \cdot \sqrt{x+y-2}}\Big)$.

Case 1. If $x = 2$, $y = 1$, then $f(2, 1) = \dfrac{\sqrt{2}}{2} \geq \dfrac{1}{\sqrt{2}} - \dfrac{1}{\sqrt{2-1}}$, so Lemma 2 holds.

Case 2. If $x = 2$, $y > 1$, then $\dfrac{\partial f}{\partial y} < 0$. Hence, $f(2, y) \geq \lim\limits_{y \to +\infty}(\dfrac{\sqrt{2+y-2}}{\sqrt{2y}} - \dfrac{\sqrt{2+y-3}}{\sqrt{(2-1)y}}) = \dfrac{1}{\sqrt{2}} - \dfrac{1}{\sqrt{2-1}}$, so Lemma 2 holds.

Case 3. Let $x \in [3, +\infty)$, $y \in [1, +\infty)$, then we have

$0 < (x^2 - x - 4)y + 2(x-2)(x-3)$

$= x^2y + 2x^2 + 12 - xy - 4y - 10x$

$= x^3y - 5x^2y + 8xy - 4y + x^4 - 8x^3 + 23x^2 - 28x + 12 - (x^3y - 6x^2y + 9xy + x^4 - 8x^3 + 21x^2 - 18x)$

$= (x-2)^2(x-1)(x+y-3) - (x-3)^2x(x+y-2)$,

which leads to

$$\frac{x-3}{\sqrt{x-1} \cdot \sqrt{x+y-3}} < \frac{x-2}{\sqrt{x} \cdot \sqrt{x+y-2}}.$$

That is, $\dfrac{\partial f}{\partial y} < 0$.

Then we have $f(x, y) \geq \lim\limits_{y \to +\infty}(\dfrac{\sqrt{x+y-2}}{\sqrt{xy}} - \dfrac{\sqrt{x+y-3}}{\sqrt{(x-1)y}}) = \dfrac{1}{\sqrt{x}} - \dfrac{1}{\sqrt{x-1}}$, so Lemma 2 holds. □

Theorem 2. Let x_1x_2 be an edge of a graph G and x_1x_2 is not an isolate edge, then $ABC(G - x_1x_2) < ABC(G)$.

Proof. Let $E_0 = E(G) \setminus \{x_1x_2\}$ and let $d(x_i) = d_i$, $i = 1, 2$. If $\min\{d_1, d_2\}$=1. Note that x_1x_2 is not an isolate edge, then we have done by Lemma 1. Otherwise we can assume

$d_1 \geq 2$ and $d_2 \geq 2$. Let us observe the function

$$f(d_1,d_2) = ABC(G) - ABC(G - x_1x_2)$$
$$= \frac{\sqrt{d_1+d_2-2}}{\sqrt{d_1d_2}} + \sum_{x_1v\in E_0} \frac{\sqrt{d_1+d_v-2}}{\sqrt{d_1d_v}} - \sum_{x_1v\in E_0} \frac{\sqrt{(d_1-1)+d_v-2}}{\sqrt{(d_1-1)d_v}}$$
$$+ \sum_{x_2u\in E_0} \frac{\sqrt{d_2+d_u-2}}{\sqrt{d_2d_u}} - \sum_{x_2u\in E_0} \frac{\sqrt{(d_2-1)+d_u-2}}{\sqrt{(d_2-1)d_u}}$$
$$= \frac{\sqrt{d_1+d_2-2}}{\sqrt{d_1d_2}} + \sum_{x_1v\in E_0} \Big(\frac{\sqrt{d_1+d_v-2}}{\sqrt{d_1d_v}} - \frac{\sqrt{d_1+d_v-3}}{\sqrt{(d_1-1)d_v}}\Big)$$
$$+ \sum_{x_2u\in E_0} \Big(\frac{\sqrt{d_2+d_u-2}}{\sqrt{d_2d_u}} - \frac{\sqrt{d_2+d_u-3}}{\sqrt{(d_2-1)d_u}}\Big).$$

By Lemma 2, we have

$$f(d_1,d_2) \geq \frac{\sqrt{d_1+d_2-2}}{\sqrt{d_1d_2}} + (d_1-1)\cdot\Big(\frac{1}{\sqrt{d_1}} - \frac{1}{\sqrt{d_1-1}}\Big) + (d_2-1)\cdot\Big(\frac{1}{\sqrt{d_2}} - \frac{1}{\sqrt{d_2-1}}\Big)$$
$$= \frac{\sqrt{d_1+d_2-2}}{\sqrt{d_1d_2}} + (d_1-1)\cdot\frac{\sqrt{d_1-1}-\sqrt{d_1}}{\sqrt{d_1}\cdot\sqrt{d_1-1}} + (d_2-1)\cdot\frac{\sqrt{d_2-1}-\sqrt{d_2}}{\sqrt{d_2}\cdot\sqrt{d_2-1}}$$
$$= \frac{\sqrt{d_1+d_2-2}}{\sqrt{d_1d_2}} + \frac{d_1-1-\sqrt{d_1(d_1-1)}}{\sqrt{d_1}} + \frac{d_2-1-\sqrt{d_2(d_2-1)}}{\sqrt{d_2}}$$
$$= \frac{\sqrt{d_1+d_2-2}}{\sqrt{d_1d_2}} + \frac{(d_1-\frac{1}{2})-\sqrt{d_1(d_1-1)}-\frac{1}{2}}{\sqrt{d_1}} + \frac{(d_2-\frac{1}{2})-\sqrt{d_2(d_2-1)}-\frac{1}{2}}{\sqrt{d_2}}$$
$$> \frac{\sqrt{d_1+d_2-2}}{\sqrt{d_1d_2}} - \frac{1}{2\sqrt{d_1}} - \frac{1}{2\sqrt{d_2}} \qquad \Big(\text{by } d_i - \frac{1}{2} > \sqrt{d_i(d_i-1)} \text{ for } i=1,2\Big)$$
$$= \frac{\sqrt{4d_1+4d_2-8} - (\sqrt{d_1}+\sqrt{d_2})}{2\sqrt{d_1d_2}}.$$

Since $2d_1+2d_2-8 \geq 0$ and $d_1+d_2 \geq 2\sqrt{d_1d_2}$, then we have

$$(2d_1+2d_2-8) + d_1 + d_2 \geq 2\sqrt{d_1d_2},$$

which leads to

$$\sqrt{4d_1+4d_2-8} \geq \sqrt{d_1} + \sqrt{d_2}.$$

That is, $f(d_1,d_2) > 0$.

Therefore $ABC(G - x_1x_2) < ABC(G)$. The proof is completed. □

By Theorem 2, the following Corollaries and Theorem are clear.

Corollary 1. Let G be a graph without isolate edges, let v be a vertex of G, then $ABC(G - v) \leq ABC(G)$, and the equality holds if and only if v is an isolated vertex of G.

Corollary 2. Let G be a graph without isolate edges and isolate vertices, let H be a subgraph of G, then $ABC(H) \leq ABC(G)$, and the equality holds if and only if $G = H$.

Theorem 3. Let G be a graph with n vertices, then $ABC(G) \leq ABC(K_n) = \frac{n}{2}\sqrt{2n-4}$, and the equality holds if and only if $G = K_n$.

Remark. By Theorem 2, it is also clear that the minimum ABC value of trees with n vertices is the minimum ABC value of all connected graphs with n vertices. But, finding the minimum ABC value of trees remains an open problem [7].

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