# On the ABC index of cacti 

Jianping Lia<br>Faculty of Applied Mathematics, Guangdong University of Technology, Guangzhou 510090, P.R. China<br>email: lijp06@gdut.edu.cn

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#### Abstract

The atom-bond connectivity ( ABC ) index is a recently introduced topological index defined as $A B C(G)=\sum_{u v \in E(G)} \sqrt{\frac{d_{u}+d_{v}-2}{d_{u} d_{v}}}$, where $d_{u}$ and $d_{v}$ are the degrees of the vertices $u$ and $v$ in the graph $G$. We determine the unique cactus with maximum ABC index among cacti with $n$ vertices, and the unique cacti with maximum $A B C$ index among cacti with $n$ vertices and $r$ cycles and among cacti with $n$ vertices and $k$ pendent vertices, respectively, where $0 \leq r \leq\left\lfloor\frac{n-1}{2}\right\rfloor$ and $0 \leq k \leq n-1$.


Keywords Atom-bond connectivity index; cacti
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## 1 Introduction

Let $G$ be a simple graph with vertex set $V(G)$ and edge set $E(G)$. For $u \in V(G), N(u)$ denotes the set of neighbors of $u$ in $G$, and the degree of $u$ is $d_{u}=|N(u)|$. The atom-bond connectivity (ABC) index of $G$ is defined as [3]

$$
A B C(G)=\sum_{u v \in E(G)} \sqrt{\frac{d_{u}+d_{v}-2}{d_{u} d_{v}}} .
$$

[^0]The ABC index displays an excellent correlation with the heat of information of alkanes [3, 2]. Furtula et al. [4] determined the minimum and maximum values of the ABC index for molecular trees (trees with maximum degree at most four) and showed that the star is the unique tree with the maximum ABC index when the number of vertices is given. Many other results of ABC index have been established $[6,7,1]$.

A cactus is a connected graph in which any two cycles have at most one vertex in common. Lu et al. [5] determined the unique cactus with minimum Randić index among cacti with $n$ vertices and $r$ cycles. In this paper, we determine the unique cactus with maximum ABC index among cacti with $n$ vertices, and the unique cacti with maximum ABC index among cacti with $n$ vertices and $r$ cycles and among cacti with $n$ vertices and $k$ pendent vertices, respectively, where $0 \leq r \leq\left\lfloor\frac{n-1}{2}\right\rfloor$ and $0 \leq k \leq n-1$.

## 2 The maximum ABC index of cacti with $n$ vertices

For $0 \leq r \leq\left\lfloor\frac{n-1}{2}\right\rfloor$, let $\mathbb{C}(n, r)$ be the set of cacti with $n$ vertices and $r$ cycles, and $C^{0}(n, r)$ the cactus obtained from $r$ triangles with a common vertex by attaching $n-2 r-1$ pendent vertices to the common vertex. Note that $\mathbb{C}(n, 0)$ and $\mathbb{C}(n, 1)$ are trees and unicyclic graphs, respectively.

Lemma 1 [4] Let $G \in \mathbb{C}(n, 0), n \geq 2$, then

$$
A B C(G) \leq \sqrt{(n-1)(n-2)}
$$

with equality if and only if $G \cong C^{0}(n, 0)$.
Lemma 2 [6] Let $G \in \mathbb{C}(n, 1), n \geq 3$, then

$$
A B C(G) \leq(n-3) \sqrt{\frac{n-2}{n-1}}+\frac{3}{\sqrt{2}}
$$

with equality if and only if $G \cong C^{0}(n, 1)$.
Lemma 3 [7] Let $f(x, y)=\sqrt{\frac{x+y-2}{x y}}=\sqrt{\frac{1}{x}+\frac{1}{y}-\frac{2}{x y}}$, where $x, y \geq 1$. If $y \geq 2$ is fixed, then $f(x, y)$ is decreasing for $x$.

The following lemma is obvious.
Lemma 4 Let $x$ be a positive integer. Denote $f(x)=\sqrt{\frac{x-1}{x}}$. Then $f(x)$ is increasing in $x$.

Note that for a vertex $v$ of a simple graph $G$ on $n$ vertices, $\sqrt{\frac{d_{v}-1}{d_{v}}} \leq \sqrt{\frac{n-2}{n-1}}$ with equality if and only if $d_{v}=n-1$. This fact will be used in our proof.

Let

$$
g(n, r)=\frac{3 r}{\sqrt{2}}+(n-2 r-1) \sqrt{\frac{n-2}{n-1}}
$$

Theorem 1 Let $G \in \mathbb{C}(n, r)$, where $0 \leq r \leq\left\lfloor\frac{n-1}{2}\right\rfloor$. Then

$$
A B C(G) \leq g(n, r)
$$

with equality if and only if $G \cong C^{0}(n, r)$.
Proof. We will prove the result by induction on $n$ and $r$. If $r=0,1$, then the theorem is true by Lemma 1 and Lemma 2. Suppose that $r \geq 2$ and then $n \geq 5$. If $n=5$, then the theorem holds trivially as there is only one graph in $\mathbb{C}(5,2)$.

Suppose that $n \geq 6, r \geq 2$. Let $G \in \mathbb{C}(n, r)$ and $\delta(G)$ be the minimum degree of $G$. By the definition of a cactus, $\delta(G)=1$ or 2 .
Case 1. $\delta(G)=1$. Let $x y \in E(G)$ with $d_{y}=1$. Let $N(x) \backslash\{y\}=\left\{x_{1}, x_{2}, \ldots, x_{d-1}\right\}$, where $d=d_{x}$. Obviously, $d \geq 2$. Suppose without loss of generality that $d_{x_{1}}=d_{x_{2}}=\cdots=d_{x_{p-1}}=$ 1 and $d_{x_{i}} \geq 2$ for $p \leq i \leq d-1$, where $p \geq 1$. Set $G^{\prime}=G-y-x_{1}-x_{2}-\cdots-x_{p-1}$ (if $p=1$, then $\left.G^{\prime}=G-y\right)$. Obviously, $G^{\prime} \in \mathbb{C}(n-p, r)$. Denote $d_{x_{i}}=d_{i}$ for $p \leq i \leq d-1$. By the induction assumption,

$$
A B C\left(G^{\prime}\right) \leq g(n-p, r)
$$

with equality if and only if $G^{\prime} \cong C^{0}(n-p, r)$. Now by Lemma 3 and Lemma 4 , we have

$$
\begin{aligned}
A B C(G) & =A B C\left(G^{\prime}\right)+p \sqrt{\frac{d-1}{d}}+\sum_{i=p}^{d-1}\left(\sqrt{\frac{d+d_{i}-2}{d d_{i}}}-\sqrt{\frac{(d-p)+d_{i}-2}{(d-p) d_{i}}}\right) \\
& \leq g(n-p, r)+p \sqrt{\frac{d-1}{d}} \\
& \leq g(n, r)+(n-p-2 r-1) \sqrt{\frac{n-p-2}{n-p-1}}-(n-2 r-1) \sqrt{\frac{n-2}{n-1}}+p \sqrt{\frac{n-2}{n-1}} \\
& =g(n, r)+(n-p-2 r-1)\left(\sqrt{\frac{n-p-2}{n-p-1}}-\sqrt{\frac{n-2}{n-1}}\right) \\
& \leq g(n, r)
\end{aligned}
$$

with equalities if and only if $G^{\prime} \cong C^{0}(n-p, r), d=n-1$, and $2 r=n-p-1$, i.e., $G \cong$ $C^{0}(n, r)$.

Case 2. $\delta(G)=2$. Then there exists an edge $v w \in E(G)$ such that $d_{v}=d_{w}=2$. Let $u$ be
the neighbor of $v$ different from $w$.
Subcase 2.1. $u w \notin E(G)$. Let $G^{\prime}=G-v+u w$. Obviously, $G^{\prime} \in \mathbb{C}(n-1, r)$. By the induction assumption, $A B C\left(G^{\prime}\right) \leq g(n-1, r)$. Then

$$
\begin{aligned}
A B C(G) & =A B C\left(G^{\prime}\right)+\frac{1}{\sqrt{2}} \leq g(n-1, r)+\frac{1}{\sqrt{2}} \\
& =g(n, r)+(n-2 r-1)\left(\sqrt{\frac{n-3}{n-2}}-\sqrt{\frac{n-2}{n-1}}\right)+\frac{1}{\sqrt{2}}-\sqrt{\frac{n-3}{n-2}} \\
& <g(n, r) .
\end{aligned}
$$

Subcase 2.2. $u w \in E(G)$. Denote $d_{u}=k$, then $k \geq 3$; Otherwise $G$ is not connected. Let $G^{\prime}=G-v-w$. Obviously, $G^{\prime} \in \mathbb{C}(n-2, r-1)$. Denote $N(u) \backslash\{v, w\}=\left\{u_{1}, u_{2}, \ldots, u_{k-2}\right\}$ and $d_{u_{i}}=k_{i}$ for $1 \leq i \leq k-2$. By the induction assumption,

$$
A B C\left(G^{\prime}\right) \leq g(n-2, r-1)
$$

with equality if and only if $G^{\prime} \cong C^{0}(n-2, r-1)$. Now by Lemmas 3 and 4 , we have

$$
\begin{aligned}
A B C(G) & =A B C\left(G^{\prime}\right)+\frac{3}{\sqrt{2}}+\sum_{i=1}^{k-2}\left(\sqrt{\frac{k+k_{i}-2}{k k_{i}}}-\sqrt{\frac{(k-2)+k_{i}-2}{(k-2) k_{i}}}\right) \\
& \leq g(n-2, r-1)+\frac{3}{\sqrt{2}} \\
& =g(n, r)+(n-2 r-1)\left(\sqrt{\frac{n-4}{n-3}}-\sqrt{\frac{n-2}{n-1}}\right) \\
& \leq g(n, r)
\end{aligned}
$$

with equalities if and only if $G^{\prime} \cong C^{0}(n-2, r-1), d=n-1$, and $2 r=n-1$, i.e., $G \cong$ $C^{0}(n, r)$.

By combining Case 1 and Case 2, the result follows.
Theorem 2 Let $G$ be a cactus with $n \geq 3$ vertices. Then

$$
A B C(G) \leq \begin{cases}\frac{3 n-3}{4} \sqrt{2} & \text { if } n \text { is odd } \\ \frac{3 n-6}{4} \sqrt{2}+\sqrt{\frac{n-2}{n-1}} & \text { if } n \text { is even }\end{cases}
$$

with equality if and only if $G \cong C^{0}\left(n,\left\lfloor\frac{n-1}{2}\right\rfloor\right)$.
Proof. Let $r$ be the number of cycles of $G$. Then $0 \leq r \leq\left\lfloor\frac{n-1}{2}\right\rfloor$. By Theorem 1, $A B C(G) \leq$ $g(n, r)$ with equality if and only if $G \cong C^{0}(n, r)$. Note that

$$
\frac{\partial g(n, r)}{\partial r}=\frac{3}{\sqrt{2}}-2 \sqrt{\frac{n-2}{n-1}}>0
$$

Then $g(n, r)$ is strictly increasing for $0 \leq r \leq\left\lfloor\frac{n-1}{2}\right\rfloor$. Thus $A B C(G) \leq g\left(n,\left\lfloor\frac{n-1}{2}\right\rfloor\right)$ with equality if and only if $G \cong C^{0}(n, r)$ with $r=\left\lfloor\frac{n-1}{2}\right\rfloor$. It is easily seen that

$$
g\left(n,\left\lfloor\frac{n-1}{2}\right\rfloor\right)= \begin{cases}\frac{3 n-3}{4} \sqrt{2} & \text { if } n \text { is odd } \\ \frac{3 n-6}{4} \sqrt{2}+\sqrt{\frac{n-2}{n-1}} & \text { if } n \text { is even. }\end{cases}
$$

The result follows.
Note that $C^{0}\left(n, \frac{n-2}{2}\right)$ has a perfect matching for even $n$. Thus we have that if $G$ is a cactus with a perfect matching on $n \geq 4$ vertices, then $A B C(G) \leq \frac{3 n-6}{4} \sqrt{2}+\sqrt{\frac{n-2}{n-1}}$ with equality if and only if $G \cong C^{0}\left(n, \frac{n-2}{2}\right)$.

## 3 The maximum ABC index of cacti with $k$ pendents

For $0 \leq k \leq n-1$, let $\mathcal{C}(n, k)$ be the set of cacti with $n$ vertices and $k$ pendents, and $H^{0}(n, k)$ the cactus obtained by adding $\frac{n-k-2}{2}$ independent edges to the star $S_{n-1}$ and then inserting a vertex of degree 2 in one of those independent edges if $n-k$ is even, and by adding $\frac{n-k-1}{2}$ independent edges to the star $S_{n}$ if $n-k$ is odd. Let

$$
\varphi(n, k)= \begin{cases}\frac{n-k-1}{2} \frac{3}{\sqrt{2}}+k \sqrt{\frac{n-2}{n-1}} & \text { if } n-k \text { is odd } \\ \frac{n-k-2}{2} \frac{3}{\sqrt{2}}+\frac{1}{\sqrt{2}}+k \sqrt{\frac{n-3}{n-2}} & \text { if } n-k \text { is even. }\end{cases}
$$

Lemma 5 Let $n \geq 3$ and $0 \leq k \leq n-2$, then

$$
\varphi(n-1, k)+\frac{1}{\sqrt{2}} \leq \varphi(n, k)
$$

with equality if and only if $n-k$ is even.
Proof. If $n-k$ is even, then $(n-1)-k$ is odd and we have

$$
\begin{aligned}
\varphi(n-1, k)+\frac{1}{\sqrt{2}} & =\frac{(n-1)-k-1}{2} \frac{3}{\sqrt{2}}+k \sqrt{\frac{n-3}{n-2}}+\frac{1}{\sqrt{2}} \\
& =\frac{n-k-2}{2} \frac{3}{\sqrt{2}}+\frac{1}{\sqrt{2}}+k \sqrt{\frac{n-3}{n-2}} \\
& =\varphi(n, k) .
\end{aligned}
$$

If $n-k$ is odd, then $(n-1)-k$ is even, and for $n \geq 4$ we have

$$
\begin{aligned}
\varphi(n-1, k)+\frac{1}{\sqrt{2}} & =\frac{n-k-1}{2} \frac{3}{\sqrt{2}}+k \sqrt{\frac{n-4}{n-3}}-\frac{1}{\sqrt{2}} \\
& =\varphi(n, k)+k\left(\sqrt{\frac{n-4}{n-3}}-\sqrt{\frac{n-2}{n-1}}\right)-\frac{1}{\sqrt{2}} \\
& <\varphi(n, k) .
\end{aligned}
$$

The case $n=3, k=0$ also holds. The result follows.

Lemma 6 Let $a$ and $b$ be two integers with $3 \leq a \leq b$ and $a+b=n$. Let $f(a, b)=$ $(a-1) \sqrt{\frac{a-1}{a}}+\sqrt{\frac{a+b-2}{a b}}+(b-1) \sqrt{\frac{b-1}{b}}$. Then $f(a, b)<f(2, n-2)$.

Proof. If $a=b$, then $n$ is even. By direct calculation, it is easily seen that $f\left(\frac{n}{2}, \frac{n}{2}\right)<$ $f(2, n-2)$.

Suppose that $a<b$. Then it suffices to show that $f(a, b)<f(a-1, b+1)$. For $3 \leq x<\frac{n}{2}$, let $l(x)=(x-1) \sqrt{\frac{x-1}{x}}+\sqrt{\frac{n-2}{x(n-x)}}+(n-x-1) \sqrt{\frac{n-x-1}{n-x}}$ and $h(x)=\frac{2 x+1}{2 x} \sqrt{\frac{x-1}{x}}$. Then $h^{\prime}(x)=\frac{1}{2 x^{2}}\left(-\sqrt{\frac{x-1}{x}}+\frac{1+2 x}{2 x} \sqrt{\frac{x}{x-1}}\right)>0$, and thus $l^{\prime}(x)=\frac{2 x+1}{2 x} \sqrt{\frac{x-1}{x}}-\frac{2(n-x)+1}{2(n-x)} \sqrt{\frac{n-x-1}{n-x}}-$ $\frac{\sqrt{n-2}}{2} \frac{n-2 x}{\left(n x-x^{2}\right)^{3 / 2}}<h(x)-h(n-x)<0$, implying that $l(x)<l(x-1)$. Thus we have $f(a, b)<$ $f(a-1, b+1)$.

Lemma 7 Let $G \in \mathcal{C}(n, 0)$. Then $\operatorname{ABC}(G) \leq \varphi(n, 0)$ with equality if and only if $G \cong$ $H^{0}(n, 0)$.

Proof. We will prove the result by induction on $n$. Since $G$ has no pendent vertices, $n \geq 3$. If $n=3,4$, then the theorem holds trivially as there is only one graph $C_{n}$ in $\mathcal{C}(3,0)$ and $\mathcal{C}(4,0)$. If $n=5$, then $G=C_{5}$ or $H^{0}(5,0)$, and the theorem holds because it is easy to check that $A B C\left(C_{5}\right)<\varphi(5,0)=A B C\left(H^{0}(5,0)\right)$. If $n=6$, then there are two graphs in $\mathcal{C}(n, k) \backslash H^{0}(6,0)$, one is the graph obtained from two vertex-disjoint triangles by adding an edge with ABC index $\frac{6}{\sqrt{2}}+\frac{2}{3}$, the other graph $C_{6}$ with ABC index $\frac{6}{\sqrt{2}}$, and both are smaller than $\varphi(6,0)$. Thus the result holds for $n=3,4,5,6$.

Suppose $n \geq 7$ and the result holds for cacti with no pendent vertices for which the number of vertices is at most $n-1$. Let $G \in \mathcal{C}(n, 0)$. Then there is an edge $w_{1} w_{2} \in E(G)$ such that $d_{w_{1}}=d_{w_{2}}=2$. Let $w_{3}$ be the neighbor of $w_{1}$ different from $w_{2}$.
Case 1. $w_{2} w_{3} \notin E(G)$. Let $G^{\prime}=G-w_{1}+w_{2} w_{3}$. Obviously, $G^{\prime} \in \mathcal{C}(n-1,0)$. By the
induction assumption and Lemma 5, we have

$$
A B C(G)=A B C\left(G^{\prime}\right)+\frac{1}{\sqrt{2}} \leq \varphi(n-1,0)+\frac{1}{\sqrt{2}} \leq \varphi(n, 0)
$$

with equality if and only if $G^{\prime} \cong H^{0}(n-1,0)$ and $n$ is even, i.e., $G \cong H^{0}(n, 0)$ for even $n$.
Case 2. $w_{2} w_{3} \in E(G)$. Denote $d_{w_{3}}=t$. Then $t \geq 3$.
Subcase 2.1. $t \geq 4$. Let $G^{\prime}=G-w_{1}-w_{2}$. Obviously, $G^{\prime} \in \mathcal{C}(n-2,0)$. Denote $N\left(w_{3}\right) \backslash$ $\left\{w_{1}, w_{2}\right\}=\left\{u_{1}, u_{2}, \ldots, u_{t-2}\right\}$ and $d_{u_{i}}=t_{i}$ for $1 \leq i \leq t-2$. Note that $n-2$ and $n$ have the same parity. By the induction assumption and Lemma 3, we have

$$
\begin{aligned}
A B C(G) & =A B C\left(G^{\prime}\right)+\frac{3}{\sqrt{2}}+\sum_{i=1}^{t-2}\left(\sqrt{\frac{t+t_{i}-2}{t t_{i}}}-\sqrt{\frac{(t-2)+t_{i}-2}{(t-2) t_{i}}}\right) \\
& \leq \varphi(n-2,0)+\frac{3}{\sqrt{2}} \\
& \leq \begin{cases}\frac{n-2-1}{2} \frac{3}{\sqrt{2}}+\frac{3}{\sqrt{2}}=\varphi(n, 0) & \text { if } n \text { is odd, } \\
\frac{n-2-2}{2} \frac{3}{\sqrt{2}}+\frac{1}{\sqrt{2}}+\frac{3}{\sqrt{2}}=\varphi(n, 0) & \text { if } n \text { is even, }\end{cases}
\end{aligned}
$$

with equality if and only if $G^{\prime} \cong H^{0}(n-2,0)$ and $t_{i}=2$ for $1 \leq i \leq t-2$, i.e., $G \cong H^{0}(n, 0)$.
Subcase 2.2. $t=3$. Then $G$ has a triangle $C=w_{1} w_{2} w_{3}$ with $d_{w_{1}}=d_{w_{2}}=2$ and $d_{w_{3}}=3$. In the following, we will prove that $\operatorname{ABC}(G)<\varphi(n, 0)$ for this subcase by contradiction. Let $G$ be a counterexample such that $n$ is as small as possible. Then $\operatorname{ABC}(G) \geq \varphi(n, 0)$. Let $z$ be the neighbor of $w_{3}$ different from $w_{1}$ and $w_{2}$. Suppose that $d_{z} \geq 3$. Let $N(z)=$ $\left\{w_{3}, z_{2}, \ldots, z_{d^{\prime}}\right\}$, where $d^{\prime}=d_{z}$. Let $G^{\prime}=G-\left\{w_{1}, w_{2}, w_{3}\right\}$ and denote $d_{z_{i}}=d_{i}^{\prime}$. Obviously, $G^{\prime} \in \mathcal{C}(n-3,0)$. Combining the choice of $G$ and the conclusion of the above subcase, we have $A B C\left(G^{\prime}\right) \leq \varphi(n-3,0)$. Hence

$$
\begin{aligned}
A B C(G) & =A B C\left(G^{\prime}\right)+\frac{3}{\sqrt{2}}+\sqrt{\frac{d^{\prime}+1}{3 d^{\prime}}}+\sum_{i=2}^{d^{\prime}}\left(\sqrt{\frac{d^{\prime}+d_{i}^{\prime}-2}{d^{\prime} d_{i}^{\prime}}}-\sqrt{\frac{\left(d^{\prime}-1\right)+d_{i}^{\prime}-2}{\left(d^{\prime}-1\right) d_{i}^{\prime}}}\right) \\
& \leq A B C\left(G^{\prime}\right)+\frac{3}{\sqrt{2}}+\sqrt{\frac{d^{\prime}+1}{3 d^{\prime}}} \\
& \leq \varphi(n-3,0)+\frac{3}{\sqrt{2}}+\sqrt{\frac{d^{\prime}+1}{3 d^{\prime}}}
\end{aligned}
$$

If $n$ is odd, then $n-3$ is even and

$$
\begin{aligned}
A B C(G) & \leq \varphi(n-3,0)+\frac{3}{\sqrt{2}}+\sqrt{\frac{d^{\prime}+1}{3 d^{\prime}}} \\
& =\frac{n-3-2}{2} \frac{3}{\sqrt{2}}+\frac{1}{\sqrt{2}}+\frac{3}{\sqrt{2}}+\sqrt{\frac{d^{\prime}+1}{3 d^{\prime}}} \\
& =\varphi(n, 0)-\frac{2}{\sqrt{2}}+\sqrt{\frac{d^{\prime}+1}{3 d^{\prime}}} \\
& <\varphi(n, 0),
\end{aligned}
$$

a contradiction. If $n$ is even, then $n-3$ is odd and

$$
\begin{aligned}
A B C(G) & \leq \varphi(n-3,0)+\frac{3}{\sqrt{2}}+\sqrt{\frac{d^{\prime}+1}{3 d^{\prime}}} \\
& =\frac{n-3-1}{2} \frac{3}{\sqrt{2}}+\frac{3}{\sqrt{2}}+\sqrt{\frac{d^{\prime}+1}{3 d^{\prime}}} \\
& =\varphi(n, 0)-\frac{1}{\sqrt{2}}+\sqrt{\frac{d^{\prime}+1}{3 d^{\prime}}} \\
& <\varphi(n, 0)
\end{aligned}
$$

a contradiction again. Suppose that $d_{z}=2$. Suppose that $G$ contains a path $P=x_{1} x_{2} x_{3} x_{4}$ with $d_{x_{2}}=d_{x_{3}}=2$. Let $G^{\prime}=G-x_{3}+x_{2} x_{4}$. Then $G^{\prime} \in \mathcal{C}(n-1,0)$ and $G^{\prime}$ contains the triangle $w_{1} w_{2} w_{3}$ with $d_{w_{1}}=d_{w_{2}}=2$ and $d_{w_{3}}=3$. By the choice of $G$, we have $A B C\left(G^{\prime}\right)<$ $\varphi(n-1,0)$. By Lemma 5, we have $A B C(G)=A B C\left(G^{\prime}\right)+\frac{1}{\sqrt{2}}<\varphi(n-1,0)+\frac{1}{\sqrt{2}} \leq \varphi(n, 0)$. Hence $\operatorname{ABC}(G)<\varphi(n, 0)$, a contradiction. Thus $G$ does not contain a path $P=x_{1} x_{2} x_{3} x_{4}$ with $d_{x_{2}}=d_{x_{3}}=2$. Thus both neighbors of $z$ are of degree at least 3 . Consider the graph $G^{\prime}=G-\left\{w_{1}, w_{2}, w_{3}, z\right\}$ which is in $\mathcal{C}(n-4,0)$. As above, we may finally have a contradiction.

Theorem 3 Let $G \in \mathcal{C}(n, k)$, where $0 \leq k \leq n-1$. Then

$$
A B C(G) \leq \begin{cases}\sqrt{(n-1)(n-2)} & \text { if } k=n-1 \\ \sqrt{2}+(n-3) \sqrt{\frac{n-3}{n-2}} & \text { if } k=n-2 \\ \varphi(n, k) & \text { if } k \leq n-3\end{cases}
$$

with equality if and only if $G \cong S_{n}$ for $k=n-1, G \cong S(2, n-2)$ for $k=n-2$, and $G \cong$ $H^{0}(n, k)$ for $k \leq n-3$, where $S(2, n-2)$ is the graph obtained by joining a vertex to one pendent vertex of the star $S_{n-1}$.

Proof. The case $k=n-1$ is obvious since in this case $G \cong S_{n}$.
Suppose $k=n-2$. Then $n \geq 4$, and $G$ is a tree with diameter three, which is obtainable from a path with two vertices by attaching $a$ pendent vertices to one end vertex and $b$ pendent vertices to the other end vertex, where $a+b=n-2$ and $a \leq b$. If $a=1$, then $G \cong S(2, n-2)$ and $A B C(G)=\sqrt{2}+(n-3) \sqrt{\frac{n-3}{n-2}}=f(2, n-2)$. If $a \geq 2$, then $A B C(G)=$ $a \sqrt{\frac{a}{a+1}}+\sqrt{\frac{a+b}{(a+1)(b+1)}}+b \sqrt{\frac{b}{b+1}}=f(a+1, b+1)<f(2, n-2)$.

Now suppose $0 \leq k \leq n-3$. We prove the result by induction on $k$. If $k=0$, then the result is true by Lemma 7 .

Suppose that $k \geq 1$ and the result holds for cacti with at most $k-1$ pendent vertices. Let $G \in \mathcal{C}(n, k)$ and $u v \in E(G)$ with $d_{u}=1$. Let $N(v)=\left\{u, v_{1}, v_{2}, \ldots, v_{d-1}\right\}$, where $d=d_{v}$. Obviously, $d \geq 2$. Suppose without loss of generality that $d_{v_{1}}=d_{v_{2}}=\cdots=d_{v_{p-1}}=1$ and $d_{v_{i}} \geq 2$ for $p \leq i \leq d-1$, where $p \geq 1$. Denote $d_{v_{i}}=d_{i}$ for $p \leq i \leq d-1$. Then set $G^{\prime}=$ $G-u-v_{1}-v_{2}-\cdots-v_{p-1}$ (if $p=1$, then $G^{\prime}=G-u$ ). Obviously, $G^{\prime} \in \mathcal{C}(n-p, k-p)$. Note that $(n-p)-(k-p)$ and $n-k$ have the same parity. By the induction assumption and Lemma 3, we have

$$
\begin{aligned}
A B C(G) & =A B C\left(G^{\prime}\right)+p \sqrt{\frac{d-1}{d}}+\sum_{i=p}^{d-1}\left(\sqrt{\frac{d+d_{i}-2}{d d_{i}}}-\sqrt{\frac{(d-p)+d_{i}-2}{(d-p) d_{i}}}\right) \\
& \leq \varphi(n-p, k-p)+p \sqrt{\frac{d-1}{d}}
\end{aligned}
$$

with equality if and only if $G^{\prime} \cong H^{0}(n-p, k-p)$. If $n-k$ is odd, then

$$
\begin{aligned}
A B C(G) & \leq \varphi(n-p, k-p)+p \sqrt{\frac{d-1}{d}} \\
& =\frac{n-k-1}{2} \frac{3}{\sqrt{2}}+(k-p) \sqrt{\frac{n-p-2}{n-p-1}}+p \sqrt{\frac{d-1}{d}} \\
& =\varphi(n, k)+(k-p)\left(\sqrt{\frac{n-p-2}{n-p-1}}-\sqrt{\frac{n-2}{n-1}}\right)+p\left(\sqrt{\frac{d-1}{d}}-\sqrt{\frac{n-2}{n-1}}\right) \\
& \leq \varphi(n, k),
\end{aligned}
$$

with equalities if and only if $G^{\prime} \cong H^{0}(n-p, k-p), d=n-1$, and $k=p$, i.e., $G \cong H^{0}(n, k)$. If $n-k$ is even, then

$$
\begin{aligned}
A B C(G) & \leq \varphi(n-p, k-p)+p \sqrt{\frac{d-1}{d}} \\
& =\frac{n-k-2}{2} \frac{3}{\sqrt{2}}+\frac{1}{\sqrt{2}}+(k-p) \sqrt{\frac{n-p-3}{n-p-2}}+p \sqrt{\frac{d-1}{d}} \\
& =\varphi(n, k)+(k-p)\left(\sqrt{\frac{n-p-3}{n-p-2}}-\sqrt{\frac{n-3}{n-2}}\right)+p\left(\sqrt{\frac{d-1}{d}}-\sqrt{\frac{n-3}{n-2}}\right) \\
& \leq \varphi(n, k),
\end{aligned}
$$

with equalities if and only if $G^{\prime} \cong H^{0}(n-p, k-p), d=n-2$, and $k=p$, i.e., $G \cong H^{0}(n, k)$.

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