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On Unicyclic Graph with Minimal Second Atom-Bond Connectivity Index

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Abstract Another version of atom-bond connectivity index was defined by Graovac and Ghorbani, and called the second atom-bond connectivity index(ABC_2), which can provide convenience for molecular feature and its extreme values are the focus of study. In this paper, by fractional comparison, we give the structural properties of the extremal graphs which attain the minimal ABC_2 index of unicyclic graphs of order n.

Keywords the second atom-bond connectivity index; unicyclic graph; fractional comparison; minimal value

MR(2010) Subject Classification 05C40; 92E10; 94C15

1. Introduction

Molecular topological indices have found wide applications in QSPR and QSAR studies, and they are one of the most active topics of the research in modern chemical graph theory [1]. On the topological indices, there are many publications [2–6]. One of the most important topological indices is the Randić index, which is aimed at the use in the modeling of the branching of the carbon-atom skeleton of alkanes, introduced by Randić [7]. But a great variety of physico-chemical properties are dependent on factors rather different than branching. In order to take this into account, in 1998 Ernesto Estrada et al. proposed the atom-bond connectivity index (ABC index for short) [8]. The ABC index of a graph $G=(V,E)$ is defined as

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

where d_u denotes the degree of vertex u of G.

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The number of vertices of G whose distance to the vertex u is smaller than the distance to the vertex v is denoted by $n_u=n_u(e|G)=|N_u(e|G)|$ and $N_u(e|G)=\{w\in V|d(w,u)<d(w,v)\}$. Analogously, $n_v=n_v(e|G)=|N_v(e|G)|$, where $N_v(e|G)=\{w\in V|d(w,v)<d(w,u)\}$, is the number of vertices of G whose distance to the vertex v is smaller than to u. A pendent vertex is a vertex of degree one and an edge of a graph is said to be pendant if one of its vertices is a pendent vertex.

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In 2010, Graovac and Ghorbani defined another version of the atom-bond connectivity index [9], and we called the second atom-bond connectivity index (ABC_2 index for short)

$$ABC_2(G) = \sum_{uv \in E} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}}$$

Lower and upper bounds for the ABC_2 index of general graphs and trees have been given in [10], and the maximum ABC_2 index of unicyclic graph also have been given in [11]. In this paper, we obtain the minimum ABC_2 index of unicyclic graph. All graphs considered in this paper are finite, undirected, simple and connected.

2. Some lemmas

We devote this paper to prove lower bound on the ABC_2 index of unicyclic graphs. The proof is based on the following elementary lemmas.

Lemma 2.1 *Let $f(x) = \frac{x-2}{x^2}$. Then $f(x)$ is a decreasing function for $x > 4$.*

Proof We have

$$f'(x) = \frac{x(4-x)}{x^4}.$$

$f'(x) = 0$ leads to $x = 4$, when $x \in (4, +\infty)$, $f'(x) < 0$. Thus $f(x)$ is a decreasing function for $x > 4$. □

Lemma 2.2 *Let $f(x) = \frac{2}{x}\sqrt{x-2}$, $x \in [3, n-1]$, n be a positive integer, and $n \geq 7$. Then $\min_{x \in [3,n-1]} f(x) = f(n-1)$.*

Proof We have

$$f'(x) = \frac{-x+4}{x^2\sqrt{x-2}}.$$

Let $f'(x) = 0$. We have $x = 4$. When $x \in [3, 4)$, for $f'(x) > 0$, $f(x)$ is an increasing function; $x \in (4, n-1]$, for $f'(x) < 0$, $f(x)$ is a decreasing function.

Note that $f(3) = f(6) = \frac{2}{3}$, $f(n-1) = \frac{2\sqrt{n-2}}{n-1}$ $(n \geq 7, n-1 \geq 6)$ and $f(x) \geq f(n-1)$. So

$$\min_{x \in [3,n-1]} f(x) = f(n-1). \quad \square$$

Lemma 2.3 ([12]) *If C_n is the cycle on n vertices. Then*

$$ABC_2(C_n) = \begin{cases} 2\sqrt{n-2} & n \text{ is even;} \\ \frac{2n\sqrt{n-3}}{n-1} & n \text{ is odd.} \end{cases}$$

Lemma 2.4 ([10]) *Let T be a tree on n vertices. Then the path P_n is the n-vertex tree with the minimum second atom-bond connectivity index.*

3. Lower bound on the ABC_2 index of unicyclic graphs

Let $G = (V, E)$ be a unicyclic graph of order n with its circuit $C_m = v_1 v_2 \cdots v_m v_1$ of length m, $T_1, T_2, \ldots, T_k$ $(0 \leq k \leq m)$ are the all nontrivial components (they are all nontrivial trees) of $G - E(C_m)$, u_i is the common vertex of T_i and C_m, $i = 1, 2, \ldots, k$. Such a unicyclic graph is denoted by $C_m^{u_1,u_2,\ldots,u_k}(T_1, T_2, \ldots, T_k)$. Specially, $G = C_n$ for $k = 0$, and if $k = 1$, we write $C_m(T_1)$ for $C_m^{u_1}(T_1)$; if $k = 1$, $n(T_1) = 2$, we write $C_m(P_1)$ for $C_m(T_1)$. Let $n(T_i) = l_i + 1$, $i = 1, 2, \ldots, k$. Then $l = l_1 + l_2 + \cdots + l_k = n - m$.

Theorem 3.1 *Let G be a connected unicyclic graph of order n ($n > 3$).*

(1) If $n = 4$, then

$$ABC_2(C_3(P_1)) \leq ABC_2(G) \tag{3.1}$$

with equality holding in (3.1) if and only if $G \cong C_3(P_1)$;

(2) If $n = 5$, then

$$ABC_2(C_3(P_2)) \leq ABC_2(G) \tag{3.2}$$

with equality holding in (3.2) if and only if $G \cong C_3(P_2)$;

(3) If $n = 6$, then

$$ABC_2(C_3(P_3)) \leq ABC_2(G) \tag{3.3}$$

with equality holding in (3.3) if and only if $G \cong C_3(P_3)$;

(4) If $n \geq 7$, then

$$ABC_2(C_n) \leq ABC_2(G) \tag{3.4}$$

with equality holding in (3.4) if and only if $G \cong C_n$.

Proof (1) If $n = 4$, then $G \cong C_4$ or $G \cong C_3(P_1)$. We have

$$ABC_2(C_3(P_1)) = \sqrt{2} + \sqrt{\frac{2}{3}} < 2\sqrt{2} = ABC_2(C_4).$$

From the above, we get the required result (3.1). Morever, the equality holds if and only if $G \cong C_3(P_1)$.

(2) If $n = 5$, then $G \cong C_5$ or $G \cong C_4(P_1)$ or $G \cong C_3(P_2)$, or $G \cong C_3^{u_1,u_2}(P_1, P_1)$.

Now we have

$$\begin{aligned} ABC_2(C_3(P_2)) = 2\sqrt{\frac{2}{3}} + \frac{\sqrt{2}+\sqrt{3}}{2} &< ABC_2(C_5) = \frac{5\sqrt{2}}{2} \\ &< ABC_2(C_4(P_1)) = 2\sqrt{2} + \frac{\sqrt{3}}{2} \\ &< ABC_2(C_3^{u_1,u_2}(P_1, P_1)) = \frac{3\sqrt{2}}{2} + \sqrt{3}. \end{aligned}$$

From the above, we get the required result (3.2). Morever, the equality holds if and only if $G \cong C_3(P_2)$.

(3) If $n = 6$, then $G \cong C_6$ or $G \cong C_3(P_3)$ or $G \cong C_4(P_2)$ or $G \cong C_5(P_1)$ or $G \cong C_3(T_3)$, or $G \cong C_3^{u_1,u_2}(P_1, P_2)$, $G \cong C_4^{u_1,u_2}(P_1, P_1)$, $G \cong C_3^{u_1,u_2,u_3}(P_1, P_1, P_1)$.

Now we have

$$\begin{aligned}ABC_2(C_3(P_3)) &= \frac{2}{3}+\frac{2\sqrt{3}+\sqrt{2}}{2}+\frac{2\sqrt{5}}{5} < ABC_2(C_6)=4\\ &< ABC_2(T_3)=\sqrt{3}+\frac{4}{\sqrt{5}}+\frac{2}{3}\\ &< ABC_2(C_4(P_2))=ABC_2(C_5(P_1))=\frac{5\sqrt{2}}{2}+\frac{2\sqrt{5}}{5}\\ &< ABC_2(C_4^{u_1,u_2}(P_1,P_1))=\sqrt{2}+\frac{4}{3}+\frac{4}{\sqrt{5}}\\ &< ABC_2(C_3^{u_1,u_2}(P_1,P_2))=\sqrt{\frac{2}{3}}+\frac{3}{\sqrt{2}}+\frac{4}{\sqrt{5}}\\ &< ABC_2(C_3^{u_1,u_2,u_3}(P_1,P_1,P_1))=\frac{3\sqrt{2}}{2}+\frac{6}{\sqrt{5}}.\end{aligned}$$

From the above, we get the required result (3.3). Morever, the equality holds if and only if $G \cong C_3(P_3)$.

(4) When $n \geq 7$, let G be a connected unicyclic graph of order n with girth m. We consider two cases: n is even or n is odd. By Lemma 2.3, we know the ABC_2 index of the cycle is different when n is even or odd. Therefore, we further divide the analysis into the following four cases of the unicyclic graph.

Case 1 n is even. In this case there are two subcases when m is even and m is odd.

Subcase 1.1 m is even. G is a connected unicyclic graph with $n \geq 7$ vertices, let edge $e = uv \in E(G)$.

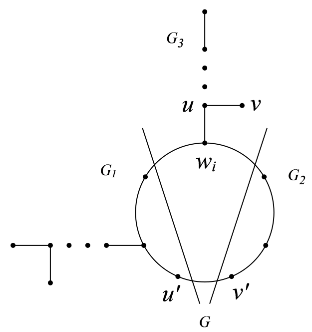

Figure 1 G: the unicycle graph

When $e = uv \in E(C_m)$, there must be a symmetric edge $e' = u'v' \in E(C_m)$ and the distance of vertex u' to u is the same as the one from the vertex v' to v, so it will have two components G_1 and G_2 for G-$\{e, e'\}$, suppose $u \in V_1 = V(G_1)$ and $v \in V_2 = V(G_2)$, $|V_1| = n_1$ and $|V_2| = n_2$, then $n_u = n_1$ and $n_v = n_2$, for edge $e = uv$, $\sqrt{\frac{n_u+n_v-2}{n_u n_v}} = \sqrt{\frac{n-2}{n_1 n_2}}$.

When $e = uv \in E(T_i)$, $G - e$ has two components G_1 and G_2, let $u \in V_1 = V(G_1)$ and $v \in V_2 = V(G_2)$, $|V_1| = n_1$ and $|V_2| = n_2$, then $n_u = n_1$ and $n_v = n_2$, for edge $e = uv$, $\sqrt{\frac{n_u+n_v-2}{n_u n_v}} = \sqrt{\frac{n-2}{n_1 n_2}}$.

Then the second atom-bond connectivity index of unicyclic graph G is as follows

$$ABC_2(G) = n\sqrt{n-2}\sqrt{\frac{1}{n_1 n_2}}.$$

Since $n_1 n_2 \leq \frac{(n_1+n_2)^2}{4} = \frac{n^2}{4}$, we have

$$ABC_2(G) = n\sqrt{n-2}\sqrt{\frac{1}{n_1 n_2}} \geq n\sqrt{n-2}\sqrt{\frac{1}{\frac{n}{2}\frac{n}{2}}} = ABC_2(C_n). \tag{3.5}$$

Above equality occurs if and only if $n_1 = n_2 = \frac{n}{2}$ holds for all $e = uv$, which implies $G \cong C_n$.

Subcase 1.2 m is odd. We consider the graph G, depicted in Figure 1. In G, for any edge $e = u'v' \in E(C_m)$, since C_m is an odd cyclic, there is a vertex w_i of C_m, whose distance to the vertex u' and v' is the same. Let $e_1, e_2 \in E(C_m)$ be the adjacent edges of vertex w_i. It will have three components G_1, G_2 and G_3 for G-$\{e, e_1, e_2\}$, suppose $u' \in V_1 = V(G_1)$, $v' \in V_2 = V(G_2)$ and $w_i \in V_3 = V(G_3)$, $|V_1| = n_{1i}$, $|V_2| = n_{2i}$ and $|V_3| = n_{0i}$, then $n_{1i} + n_{2i} + n_{0i} = n$, and any vertex of V_3 does not belong to $N_u(e|G)$ or $N_v(e|G)$, $N_u(e|G) = V_1$, $N_v(e|G) = V_2$. On the other hand, for any edge $e = uv \in E(T_i)$ we have $n_u + n_v = n$. Thus

$$ABC_2(G) = \sum_{uv \in E(T_i)} \sqrt{\frac{n-2}{n_u n_v}} + \sum_{u'v' \in E(C_m)} \sqrt{\frac{n - n_{0i} - 2}{n_{1i} n_{2i}}}.$$

Use the same way as Subcase 1.1, we can show that

$$\sqrt{\frac{1}{n_u n_v}} \geq \sqrt{\frac{1}{\frac{n}{2}\frac{n}{2}}}$$

with equality holding if and only if $n_u = n_v = \frac{n}{2}$.

In addition, we can prove that

$$\sqrt{\frac{n - n_{0i} - 2}{n_{1i} n_{2i}}} > \sqrt{\frac{n-2}{\frac{n}{2}\frac{n}{2}}},$$

that is

$$\frac{n - n_{0i} - 2}{4 n_{1i} n_{2i}} \geq \frac{n - n_{0i} - 2}{(n - n_{0i})^2} > \frac{n-2}{n^2}.$$

In order to prove the above conclusion, we use $n_{1i} n_{2i} \leq \frac{(n_{1i}+n_{2i})^2}{4} = \frac{(n-n_{0i})^2}{4}$, so

$$\frac{n - n_{0i} - 2}{4 n_{1i} n_{2i}} \geq \frac{n - n_{0i} - 2}{(n - n_{0i})^2}.$$

By Lemma 2.1, we have $\frac{n-n_{0i}-2}{(n-n_{0i})^2} > \frac{n-2}{n^2}$. Thus

$$\sqrt{\frac{n - n_{0i} - 2}{n_{1i} n_{2i}}} > \sqrt{\frac{n-2}{\frac{n}{2}\frac{n}{2}}}.$$

From the above, we conclude that

$$\begin{aligned} ABC_2(G) &= (n-m)\sqrt{n-2}\sqrt{\frac{1}{n_u n_v}} + m\sqrt{\frac{n-n_{0i}-2}{n_{1i}n_{2i}}} \\ &\geq (n-m)\sqrt{n-2}\sqrt{\frac{1}{\frac{n}{2}\frac{n}{2}}} + m\sqrt{n-2}\sqrt{\frac{1}{\frac{n}{2}\frac{n}{2}}} \\ &= 2\sqrt{n-2} = ABC_2(C_n) \end{aligned} \tag{3.6}$$

with equality holding if and only if $n_u = n_v = n_{1i} = n_{2i} = \frac{n}{2}$, $n_{0i} = 1$, which implies $G \cong C_n$.

Case 2 n is odd. In this case also there are two subcases when m is even and m is odd.

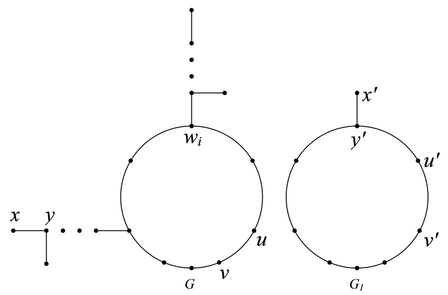

Figure 2 G: the unicycle graph, G_1: the unicyclic graph of $C_{n-1}(P1)$

Subcase 2.1 m is even. We consider the graph G and G_1, depicted in Figure 2.

Since m is even, $n \geq m+1$. When $n = m+1$, then $G = G_1 = C_{n-1}(P_1)$.

$$\begin{aligned} ABC_2(C_{n-1}(P_1)) &= \sqrt{\frac{n-2}{n-1}} + \sum_{u'v' \in E(C_{n-1})} \sqrt{\frac{n_{u'}+n_{v'}-2}{n_{u'}n_{v'}}} \\ &= \sqrt{\frac{n-2}{n-1}} + (n-1)\sqrt{n-2}\sqrt{\frac{1}{\frac{n-1}{2}\frac{n+1}{2}}}. \end{aligned}$$

When $n > m+1$, there is at least a pendant edge xy and

$$\sqrt{\frac{n_x+n_y-2}{n_x n_y}} = \sqrt{\frac{n-2}{n-1}}$$

for any edge $uv \in E(G)\backslash\{xy\}$. Since m is even, we have

$$\sqrt{\frac{n_u+n_v-2}{n_u n_v}} = \sqrt{\frac{n-2}{n_u n_v}}, \quad n_u + n_v = n.$$

Then

$$ABC_2(G) = \sqrt{\frac{n-2}{n-1}} + (n-1)\sqrt{n-2}\sqrt{\frac{1}{n_u n_v}}.$$

Since $n_u + n_v = n$ and n is odd, obviously, $\frac{1}{n_u n_v} \geq \frac{1}{\frac{n-1}{2}\frac{n+1}{2}}$. Thus

$$\begin{aligned} ABC_2(G) &\geq \sqrt{\frac{n-2}{n-1}} + (n-1)\sqrt{n-2}\sqrt{\frac{1}{\frac{n-1}{2}\frac{n+1}{2}}} \\ &= ABC_2(C_{n-1}(P_1)) \end{aligned}$$

with equality holding if and only if $n_u = \frac{n-1}{2}$, $n_v = \frac{n+1}{2}$, which implies $G \cong C_{n-1}(P_1)$.

Next, we need to prove $ABC_2(C_{n-1}(P_1)) > ABC_2(C_n)$, that is

$$\sqrt{\frac{n-2}{n-1}} + (n-1)\sqrt{n-2}\sqrt{\frac{1}{\frac{n-1}{2}\frac{n+1}{2}}} > n\sqrt{\frac{n-1-2}{\frac{n-1}{2}\frac{n-1}{2}}}. \tag{3.7}$$

We know that

$$\sqrt{\frac{n-2}{n-1}} = \sqrt{\frac{n+1}{4}\frac{n-2}{\frac{n-1}{2}\frac{n+1}{2}}} = \frac{\sqrt{n+1}}{2}\sqrt{\frac{n-2}{\frac{n-1}{2}\frac{n+1}{2}}}.$$

So, inequality (3.7) is equivalent to

$$(\frac{\sqrt{n+1}}{2} + n - 1)\sqrt{\frac{n-2}{\frac{n-1}{2}\frac{n+1}{2}}} > n\sqrt{\frac{n-3}{\frac{n-1}{2}\frac{n-1}{2}}},$$

$$(\frac{\sqrt{n+1}}{2} + n - 1)\sqrt{\frac{n-1}{n+1}}\sqrt{\frac{n-2}{\frac{n-1}{2}\frac{n-1}{2}}} > n\sqrt{\frac{n-3}{\frac{n-1}{2}\frac{n-1}{2}}},$$

$$(\frac{\sqrt{n+1}}{2} + n - 1)\sqrt{\frac{n-1}{n+1}} > n,$$

$$(n-1)\sqrt{\frac{n-1}{n+1}} > n - \frac{\sqrt{n-1}}{2},$$

$$(n+1)\sqrt{n-1} > (n-3).$$

It is clearly established ($n \geq 7$). Thus

$$ABC_2(C_{n-1}(P_1)) = \sqrt{\frac{n-2}{n-1}} + (n-1)\sqrt{n-2}\sqrt{\frac{1}{\frac{n-1}{2}\frac{n+1}{2}}}$$
$$> n\sqrt{\frac{n-3}{\frac{n-1}{2}\frac{n+1}{2}}} = ABC_2(C_n).$$

In conclusion, we know that

$$ABC_2(G) \geq ABC_2(C_{n-1}(P_1)) > ABC_2(C_n).$$

Therefore

$$ABC_2(G) \geq ABC_2(C_n) \tag{3.8}$$

with equality holding if and only if $G \cong C_n$.

Subcase 2.2 m is odd. We consider the graph G depicted in Figure 1.

Since m is odd, $n \geq m$; When $n = m$, then $G = C_n$,

$$ABC_2(C_n) = n\sqrt{\frac{n-1-2}{\frac{n-1}{2}\frac{n-1}{2}}}.$$

When $n > m$, there is at least a pendant edge xy and

$$\sqrt{\frac{n_x + n_y - 2}{n_x n_y}} = \sqrt{\frac{n-2}{n-1}}.$$

For any $e = u'v' \in E(C_m)$, let $n_{u'} = n_{1i}$, $n_{v'} = n_{2i}$, and $n - (n_{u'} + n_{v'}) = n_{0i}$. We have

$$\sqrt{\frac{n_{u'} + n_{v'} - 2}{n_{u'}n_{v'}}} = \sqrt{\frac{n - n_{0i} - 2}{n_{1i}n_{2i}}}.$$

Thus

$$\begin{aligned} ABC_2(G) &= \sqrt{\frac{n-2}{n-1}} + \sum_{uv \in E(T_i - xy)} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}} + \sum_{u'v' \in E(C_m)} \sqrt{\frac{n_{u'} + n_{v'} - 2}{n_{u'}n_{v'}}} \\ &= \sqrt{\frac{n-2}{n-1}} + (n-m-1)\sqrt{\frac{n-2}{n_u n_v}} + m\sqrt{\frac{n - n_{0i} - 2}{n_{1i}n_{2i}}}. \end{aligned}$$

Since $n_u + n_v = n$ and n is odd. Obviously,

$$\frac{1}{n_u n_v} \geq \frac{1}{\frac{n-1}{2}\frac{n+1}{2}}.$$

In addition, $n_{1i}n_{2i} \leq (\frac{n_{1i}+n_{2i}}{2})^2 = (\frac{n-n_{0i}}{2})^2$, so

$$\sqrt{\frac{n - n_{0i} - 2}{n_{1i}n_{2i}}} \geq \sqrt{\frac{n - n_{0i} - 2}{(\frac{n-n_{0i}}{2})^2}} = \frac{2}{n - n_{0i}}\sqrt{(n - n_{0i}) - 2}.$$

By Lemma 2.2, we know

$$\sqrt{\frac{n - n_{0i} - 2}{(\frac{n-n_{0i}}{2})^2}} \geq \sqrt{\frac{n-1-2}{(\frac{n-1}{2})^2}}.$$

It means that

$$\sqrt{\frac{n - n_{0i} - 2}{n_{1i}n_{2i}}} \geq \sqrt{\frac{n-1-2}{(\frac{n-1}{2})^2}}$$

with equality holding if and only if $n_{0i} = 1$, $n_{1i} = n_{2i} = \frac{n-1}{2}$.

Next we can prove

$$\frac{n-1-2}{(\frac{n-1}{2})^2} > \frac{n-2}{\frac{n-1}{2}\frac{n+1}{2}}$$

that is

$$\frac{n-1-2}{n-1} > \frac{n-2}{n+1}, \quad \frac{2}{n-1} < \frac{3}{n+1}, \quad n > 5.$$

It is obvious ($n \geq 7$).

As is above, we show that

$$\begin{cases} \frac{1}{n_u n_v} \geq \frac{1}{\frac{n-1}{2}\frac{n+1}{2}}, \\ \frac{n-n_{0i}-2}{n_{1i}n_{2i}} > \frac{n-2}{\frac{n-1}{2}\frac{n+1}{2}}. \end{cases}$$

To sum up

$$\begin{aligned}
ABC_2(G) &= \sqrt{\frac{n-2}{n-1}} + (n-m-1)\sqrt{\frac{n-2}{n_u n_v}} + m\sqrt{\frac{n-n_{0i}-2}{n_{1i}n_{2i}}} \\
&> \sqrt{\frac{n-2}{n-1}} + (n-m-1)\sqrt{\frac{n-2}{\frac{n-1}{2}\frac{n+1}{2}}} + m\sqrt{\frac{n-2}{\frac{n-1}{2}\frac{n+1}{2}}} \\
&= \sqrt{\frac{n-2}{n-1}} + (n-1)\sqrt{\frac{n-2}{\frac{n-1}{2}\frac{n+1}{2}}} \\
&= ABC_2(C_{n-1}(P_1)).
\end{aligned}$$

Meanwhile, using Subcase 2.1 (3.7) gives

$$\begin{aligned}
ABC_2(C_{n-1}(P_1)) &= \sqrt{\frac{n-2}{n-1}} + (n-1)\sqrt{n-2}\sqrt{\frac{1}{\frac{n-1}{2}\frac{n+1}{2}}} \\
&> n\sqrt{\frac{n-1-2}{\frac{n-1}{2}.\frac{n-1}{2}}} = ABC_2(C_n).
\end{aligned}$$

In conclusion, we know that $ABC_2(G) \geq ABC_2(C_{n-1}(P_1)) > ABC_2(C_n)$. Therefore

$$ABC_2(G) \geq ABC_2(C_n) \tag{3.9}$$

with equality holding if and only if $G \cong C_n$.

Using the above results with (3.5), (3.6), (3.8), (3.9), we get the required result. This completes the proof of the theorem. □

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