MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **91** (2024) 513–532
ISSN: 0340–6253
doi: 10.46793/match.91-2.513S

On Bicyclic Graphs with Maximal Graovac-Ghorbani Index

Rui Song[a,b], **Saihua Liu**[c,*], **Jianping Ou**[c], **Jianbin Cui**[a,b]

[a] *School of Mathematics and Information Engineering, Longdong University, Qingyang, Gansu 745000, P.R.China*

[b] *Institute of Applied Mathematics, Longdong University, Qingyang, Gansu 745000, P.R.China*

[c] *Department of Mathematics, Wuyi University, Jiangmen, Guangdong 529020, P.R.China*

`15819931748@163.com`, `lsh1808@163.com`,
`oujp@263.net`, `363555701@qq.com`

(Received June 28, 2023)

Abstract

Graovac-Ghorbani index is a new version of the atom-bond connectivity index. D. Pacheco et al. [MATCH Commun. Math. Comput. Chem. 86 (2021) 429-448] conjectured a sharp lower and upper bounds to the Graovac-Ghorbani index for all bicyclic graphs. Motivated by their nice work, in this paper we determine the maximal Graovac-Ghorbani index of bicyclic graphs and characterize the corresponding extremal graphs, which solves one of their Conjectures.

1 Introduction

Molecular descriptors play a significant role in mathematical chemistry especially in the QSPR/QSAR investigations. Among them, special place is reserved for so-called topological index [6], where topological index are numbers associated with chemical structures as a tool for compact and

*Corresponding author.

effective description of structural formulas used to study and predict the structure-property correlation of organic compounds [1, 15, 17, 22]. It is known that connectivity index has a widely application [19]. In [8], Estrada et al. proposed the concept of atom-bond connectivity index (ABC index) of a simple undirected graph G as

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

where $E(G)$ is the edge set of graph G and d_u is the degree of vertex u. About ABC index, it has proven to be a valuable predictive index in study of the heat of formation in alkanes [7, 8]. Many mathematical properties of this index are reported in [2–4, 9, 12, 16, 23–25].

In [14], Graovac and Ghorbani defined a new version of the atom-bond connectivity index as follows:

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

where the summation goes over all edges in graph G, n_u denotes the number of vertices of G whose distances to vertex u are smaller than those to other vertex v of the edge $e = uv$, and n_v defines similarly. This index is also called the second atom-bond connectivity index of graph G and is labeled as $ABC_2(G)$ [5, 13, 14, 20, 21]. In [11], Boris Furtula denoted this index as ABC_{GG} and called it Graovac-Ghorbani index because of their essential difference. Therefore, this index is denoted as ABC_{GG} and is called Graovac-Ghorbani index in this paper. In the chemistry applications, ABC_{GG} is used to model both the boiling point and melting point of the molecules. Hence, it is also applied to the pharmaceutical field. There are already many published papers on its mathematical properties [5, 10, 11, 13, 14, 20, 21]. In [18], D. Pacheco et al. determined the extremal graph with minimum Graovac-Ghorbani index among all bicyclic graphs with no pendent vertices. Additionally, they conjectured a sharp lower and upper bounds to the Graovac-Ghorbani index for all bicyclic graphs. In this paper, we determine the maximal ABC_{GG} index of bicyclic graphs and characterize the extremal graphs.

2 Preliminaries

In this section we will present two lemmas. For two real numbers $x, y \geq 1$ and integer $a \geq 2$, let $f(x,y) = \sqrt{\frac{x+y-2}{xy}}$, $g_a(x) = f(x,a) - f(x,a-1)$. Then

$$\begin{aligned} g_a(x) &= f(x,a) - f(x,a-1) \\ &= \frac{2-x}{\sqrt{a(a-1)x}(\sqrt{(a-1)(x+a-2)} + \sqrt{a(x+a-3)})}. \end{aligned}$$

In [24] R. Xing et al. showed the following lemma.

Lemma 2.1 ([24]). *$f(x,1) = \sqrt{\frac{x-1}{x}}$ is strictly increasing for x, $f(x,2) = \sqrt{\frac{1}{2}}$, and if $y \geq 3$, then $f(x,y)$ is strictly decreasing for x.*

By Lemma 2.1, we have the following Lemma 2.2, part of which has been given in [23, 24], so we omit its proof herein.

Lemma 2.2 ([23, 24]). *If $a \geq 2$, then $g_a(x) \leq g_a(2) \leq g_a(1)$ for $x \geq 2$; and for fixed x, $g_a(x)$ is strictly decreasing for a if $x = 1$, and strictly increasing for a if $x \geq 3$.*

3 Bicyclic graphs with maximum ABC_{GG} index

Let $B_{n,p}$ be the set of bicyclic graphs with n vertices and p pendent vertices. Clearly, we have that $0 \leq p \leq n-4$. Let $S(m_1, \cdots, m_k)$ be the unicyclic graph with cycle $v_1 v_2 \cdots v_k v_1$ and m_i pendent vertices adjacent to vertex v_i for all $i = 1, 2, \cdots, k$. Let $S_n^{r,t}(m_1, \cdots, m_{r-1}, n_1, \cdots, n_{t-1}, m_0)$ be a bicyclic graph shown in Figure 1. In particular, $S_n^{3,3}(m_1, n_1, m_0) = S_n^{3,3}(m_1, 0, n_1, 0, m_0)$.

Part of the following Lemma 3.1 has been shown in [5].

Lemma 3.1. *Let x, n be two positive integers with $1 \leq x \leq n-6$.*

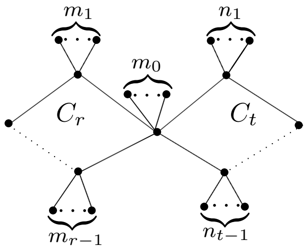

Figure 1. $S_n^{r,t}(m_1, m_2, ..., m_{r-1}, n_1, n_2, ..., n_{t-1}, m_0)$

(1) If $n = 7$, $x = 1$, then

$$\sqrt{\frac{x}{x+1}} + \sqrt{\frac{n-3-x}{n-2-x}} + \sqrt{\frac{n-3}{(x+1)(n-2-x)}} = \sqrt{\frac{3}{4}} + \sqrt{2}.$$

(2) If $n = 8$, then

$$\sqrt{\frac{x}{x+1}} + \sqrt{\frac{n-3-x}{n-2-x}} + \sqrt{\frac{n-3}{(x+1)(n-2-x)}} \leq \sqrt{\frac{2}{3}} + \sqrt{\frac{3}{4}} + \sqrt{\frac{5}{12}},$$

with equality holding if and only if $x = 2$.

(3) If $n = 9$, then

$$\sqrt{\frac{x}{x+1}} + \sqrt{\frac{n-3-x}{n-2-x}} + \sqrt{\frac{n-3}{(x+1)(n-2-x)}} \leq \sqrt{3} + \sqrt{\frac{3}{8}},$$

with equality holding if and only if $x = 3$.

(4) If $10 \leq n \leq 15$, then

$$\begin{aligned} & \sqrt{\frac{x}{x+1}} + \sqrt{\frac{n-3-x}{n-2-x}} + \sqrt{\frac{n-3}{(x+1)(n-2-x)}} \\ \leq \quad & \sqrt{\frac{2}{3}} + \sqrt{\frac{n-5}{n-4}} + \sqrt{\frac{n-3}{3(n-4)}}, \end{aligned}$$

with equality holding if and only if $x = 2$.

(5) If $n \geq 16$ *, then*

$$\sqrt{\frac{x}{x+1}} + \sqrt{\frac{n-3-x}{n-2-x}} + \sqrt{\frac{n-3}{(x+1)(n-2-x)}} \leq \sqrt{2} + \sqrt{\frac{n-4}{n-3}}$$

with equality holding if and only if $x = 1$*.*

Proof. Let $f(n,x) = \sqrt{\frac{x}{x+1}} + \sqrt{\frac{n-3-x}{n-2-x}} + \sqrt{\frac{n-3}{(x+1)(n-2-x)}}$. Thus (1) follows by direct calculation. If $n = 8$ then $x = 1$ or 2, (2) follows by comparing $f(8,1)$ and $f(8,2)$. If $n = 9$ then $x = 1, 2$ or 3, (3) also follows by comparing $f(9,1)$, $f(9,2)$ and $f(9,3)$. Next we need only prove the case $n \geq 10$.

Notice that $f(n,x) = f(n, n-3-x)$ for $x \in [1, n-4]$. In [[5], Theorem 2.4], the authors show that for $\frac{n-3}{2} \leq x \leq n-4$, if $10 \leq n \leq 15$ then $f(n,x) \leq \sqrt{\frac{2}{3}} + \sqrt{\frac{n-5}{n-4}} + \sqrt{\frac{n-3}{3(n-4)}} = f(n, n-5)$; if $n \geq 16$ then $f(n,x) \leq \sqrt{2} + \sqrt{\frac{n-4}{n-3}} = f(n, n-4)$. The above discussion shows that for all x with $1 \leq x \leq n-6$, if $10 \leq n \leq 15$ then $f(n,x) \leq \sqrt{\frac{2}{3}} + \sqrt{\frac{n-5}{n-4}} + \sqrt{\frac{n-3}{3(n-4)}} = f(n, n-5) = f(n, 2)$; if $n \geq 16$ then $f(n,x) \leq \sqrt{2} + \sqrt{\frac{n-4}{n-3}} = f(n, n-4) = f(n, 1)$. Hence, (4) and (5) follow. ■

Edge-lifting transformation on edge uv **of graph** G [5]. Let uv be a cut edge of a connected graph G but uv be not a pendent edge. We delete edge uv from G at first, then identify vertices u and v, and finally attach a new isolated vertex to this identified vertex to obtain a new graph. This graph transformation is called an edge-lifting transformation on edge uv of graph G. This transformation is pictured in Figure 2.

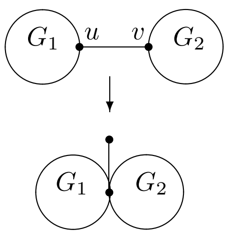

Figure 2. Edge-lifting transformation

In [5], K. C. Das et al. prove the following lemma for the case when G is a unicyclic graph. Here, we generalize it to connected graphs.

Lemma 3.2. *If G' is the graph obtained by performing edge-lifting transformation on edge uv of graph G, then*

$$ABC_{GG}(G) < ABC_{GG}(G').$$

Proof. If $xy \in E(G_1) \cup E(G_2)$ (refer to Figure 2), by the definition of ABC_{GG} index we have that

$$\sqrt{\frac{n_x + n_y - 2}{n_x n_y}}$$

contributes the same to $ABC_{GG}(G)$ and $ABC_{GG}(G')$. Since $|G_1| \geq 2$, $|G_2| \geq 2$ and $|G_1| + |G_2| = |G|$, we have

$$ABC_{GG}(G) - ABC_{GG}(G') = \sqrt{\frac{|G_1| + |G_2| - 2}{|G_1||G_2|}} - \sqrt{\frac{|G| - 2}{(|G| - 1) \cdot 1}} < 0.$$

Thus, $ABC_{GG}(G) < ABC_{GG}(G')$. ∎

Let $S_n^{r,t}$ be the set of such bicyclic graphs of order n that have two cycles with length r and t, respectively. Furthermore, these two cycles have unique common vertex.

Lemma 3.3. *If $G \in S_n^{r,t}$ is a connected bicyclic graph of order $n \geq 7$ and $r + t \geq 7$, then*

$$ABC_{GG}(G) \leq (n - 5)\sqrt{\frac{n - 2}{n - 1}} + 6\sqrt{\frac{1}{2}},$$

with the equality holding only if $G = S_n^{3,3}(m_1, m_2, n_1, n_2, m_0)$ for some integers $m_1, m_2, n_1, n_2, m_0 \geq 0$.

Proof. If G is not isomorphic to any $S_n^{r,t}(m_1, \cdots, m_{r-1}, n_1, \cdots, n_{t-1}, m_0)$, then G has a non-pendent edge uv that $uv \notin E(C_r) \cup E(C_t)$, where C_r and C_t are the two cycles of graph G. By performing edge-lifting transformation on edge uv of G we obtained a new graph G_1. From Lemma 3.2

it follows that $ABC_{GG}(G) < ABC_{GG}(G_1)$. So, we may assume in what follows that $G = S_n^{r,t}(m_1, \cdots, m_{r-1}, n_1, \cdots, n_{t-1}, m_0)$ for some integers $r, t \geq 3$. Now, two different cases occur.

Case 1. $r > 3$, $t > 3$. In this case, G has $n - r - t + 1 \leq n - 7$ pendent edges and at least $r + t \geq 8$ non-pendent edges. Since $r > 3$, $t > 3$, for each non-pendent edge $uv \in E(C_r) \cup E(C_t)$ we have $n_u \geq 2$ and $n_v \geq 2$. By Lemma 2.1, $\sqrt{\frac{n_u+n_v-2}{n_u n_v}} \leq \sqrt{\frac{1}{2}} < \sqrt{\frac{n-2}{n-1}}$ since $n \geq 7$ in this case. For any pendent edge $uv \in E(G)$, $\sqrt{\frac{n_u+n_v-2}{n_u n_v}} = \sqrt{\frac{n-2}{n-1}}$. Hence,

$$\begin{aligned} ABC_{GG}(G) &= \sum_{\substack{uv \in E(G) \\ d_u = 1}} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}} + \sum_{\substack{uv \in E(G) \\ d_u, d_v \neq 1}} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}} \\ &\leq (n - r - t + 1)\sqrt{\frac{n-2}{n-1}} + (r + t)\sqrt{\frac{1}{2}} \\ &= (n-5)\sqrt{\frac{n-2}{n-1}} + (6 - r - t)\sqrt{\frac{n-2}{n-1}} + (r + t)\sqrt{\frac{1}{2}} \\ &< (n-5)\sqrt{\frac{n-2}{n-1}} + 6\sqrt{\frac{1}{2}}. \end{aligned}$$

Case 2. $r > 3$, $t = 3$(the case when $t > 3$, $r = 3$ is similar). If $n_1, n_2 \geq 1$, then the above inequality is also true; If $n_1, n_2 = 0$, since $r \geq 4$ it follows that $(r-6)\sqrt{\frac{1}{2}} - (r-5)\sqrt{\frac{n-2}{n-1}} < 0$. Recalling $\sqrt{\frac{1}{2}} < \sqrt{\frac{n-2}{n-1}}$, we deduce that

$$\begin{aligned} ABC_{GG}(G) &= \sum_{uv \in E(C_r)} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}} + 2\sqrt{\frac{n-3}{n-2}} \\ &\quad + (n - r - 2)\sqrt{\frac{n-2}{n-1}} \\ &\leq r\sqrt{\frac{1}{2}} + 2\sqrt{\frac{n-3}{n-2}} - (r-3)\sqrt{\frac{n-2}{n-1}} + (n-5)\sqrt{\frac{n-2}{n-1}} \\ &< 6\sqrt{\frac{1}{2}} + (r-6)\sqrt{\frac{1}{2}} - (r-5)\sqrt{\frac{n-2}{n-1}} + (n-5)\sqrt{\frac{n-2}{n-1}} \\ &< (n-5)\sqrt{\frac{n-2}{n-1}} + 6\sqrt{\frac{1}{2}}. \end{aligned}$$

Finally, if $n_1 \geq 1, n_2 = 0$, then

$$\sqrt{\frac{n-3}{(n_1+1)(n-n_1-2)}} \leq \sqrt{\frac{1}{2}} \leq \sqrt{\frac{n_1}{n_1+1}} < \sqrt{\frac{n-2}{n-1}},$$

and

$$\sqrt{\frac{n-n_1-3}{n-n_1-2}} < \sqrt{\frac{n-2}{n-1}}.$$

When $r \geq 5$ we have

$$\begin{aligned} ABC_{GG}(G) &= \sum_{uv \in E(C_r)} \sqrt{\frac{n_u+n_v-2}{n_u n_v}} + \sqrt{\frac{n-3}{(n_1+1)(n-n_1-2)}} \\ &\quad + \sqrt{\frac{n_1}{n_1+1}} + \sqrt{\frac{n-n_1-3}{n-n_1-2}} + (n-r-2)\sqrt{\frac{n-2}{n-1}} \\ &< r\sqrt{\frac{1}{2}} + \sqrt{\frac{1}{2}} + 2\sqrt{\frac{n-2}{n-1}} + (n-r-2)\sqrt{\frac{n-2}{n-1}} \\ &= 6\sqrt{\frac{1}{2}} + (r-5)\sqrt{\frac{1}{2}} - (r-5)\sqrt{\frac{n-2}{n-1}} + (n-5)\sqrt{\frac{n-2}{n-1}} \\ &\leq (n-5)\sqrt{\frac{n-2}{n-1}} + 6\sqrt{\frac{1}{2}}. \end{aligned}$$

When $r = 4$, let $f(x) = \sqrt{\frac{x}{x+1}} + \sqrt{\frac{n-3-x}{n-2-x}} + \sqrt{\frac{n-3}{(x+1)(n-2-x)}}$, where $1 \leq x \leq n-6$ and $n \geq 7$. By Lemma 3.1, if $n = 7$ and $x = 1$, then $f(1) = \sqrt{2} + \sqrt{\frac{3}{4}} < \sqrt{2} + \sqrt{\frac{5}{6}}$; if $n = 8$, then $f(x) \leq f(2) = \sqrt{\frac{2}{3}} + \sqrt{\frac{3}{4}} + \sqrt{\frac{5}{12}} \approx 2.3280 < \sqrt{2} + \sqrt{\frac{6}{7}} \approx 2.3400$; if $n = 9$, then $f(x) \leq f(3) = \sqrt{3} + \sqrt{\frac{3}{8}} \approx 2.3444 < \sqrt{2} + \sqrt{\frac{7}{8}} \approx 2.3496$; if $10 \leq n \leq 15$, then $f(x) \leq f(2) = \sqrt{\frac{2}{3}} + \sqrt{\frac{n-5}{n-4}} + \sqrt{\frac{n-3}{3(n-4)}}$. Let $g(n) = \sqrt{\frac{2}{3}} + \sqrt{\frac{n-5}{n-4}} + \sqrt{\frac{n-3}{3(n-4)}} - \sqrt{2} - \sqrt{\frac{n-2}{n-1}}$. Then $g(10) = \sqrt{\frac{2}{3}} + \sqrt{\frac{5}{6}} + \sqrt{\frac{7}{18}} - \sqrt{2} - \sqrt{\frac{8}{9}} \approx -0.0040 < 0$, $g(11) = \sqrt{\frac{2}{3}} + \sqrt{\frac{6}{7}} + \sqrt{\frac{8}{21}} - \sqrt{2} - \sqrt{\frac{9}{10}} \approx -0.0034 < 0$, $g(12) = \sqrt{\frac{2}{3}} + \sqrt{\frac{7}{8}} + \sqrt{\frac{9}{24}} - \sqrt{2} - \sqrt{\frac{10}{11}} \approx -0.0034 < 0$, $g(13) = \sqrt{\frac{2}{3}} + \sqrt{\frac{8}{9}} + \sqrt{\frac{10}{27}} - \sqrt{2} - \sqrt{\frac{11}{12}} \approx -0.0038 < 0$, $g(14) = \sqrt{\frac{2}{3}} + \sqrt{\frac{9}{10}} + \sqrt{\frac{11}{30}} - \sqrt{2} - \sqrt{\frac{12}{13}} \approx -0.0043 < 0$, $g(15) = \sqrt{\frac{2}{3}} + \sqrt{\frac{10}{11}} + \sqrt{\frac{12}{33}} - \sqrt{2} - \sqrt{\frac{13}{14}} \approx -0.0049 < 0$; if $n \geq 16$, then

$f(x) \leq f(1) = \sqrt{2} + \sqrt{\frac{n-4}{n-3}} < \sqrt{2} + \sqrt{\frac{n-2}{n-1}}$. Hence, $f(x) < \sqrt{2} + \sqrt{\frac{n-2}{n-1}}$ for all x with $1 \leq x \leq n-6$. So,

$$\begin{aligned}
ABC_{GG}(G) &= \sum_{uv \in E(C_r)} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}} + \sqrt{\frac{n-3}{(n_1+1)(n-n_1-2)}} \\
&\quad + \sqrt{\frac{n_1}{n_1+1}} + \sqrt{\frac{n-n_1-3}{n-n_1-2}} + (n-r-2)\sqrt{\frac{n-2}{n-1}} \\
&\leq 6\sqrt{\frac{1}{2}} + (n-5)\sqrt{\frac{n-2}{n-1}} + \sqrt{\frac{n-3}{(n_1+1)(n-n_1-2)}} \\
&\quad + \sqrt{\frac{n_1}{n_1+1}} + \sqrt{\frac{n-n_1-3}{n-n_1-2}} - 2\sqrt{\frac{1}{2}} - \sqrt{\frac{n-2}{n-1}} \\
&< (n-5)\sqrt{\frac{n-2}{n-1}} + 6\sqrt{\frac{1}{2}}.
\end{aligned}$$

The proof is finished. ■

Lemma 3.4. *If* $G \in S_n^{3,3}(m_1, m_2, n_1, n_2, m_0)$ *has maximal* ABC_{GG} *index, then* $\min\{m_1, m_2\} = 0$ *and* $\min\{n_1, n_2\} = 0$.

Proof. If $n \leq 6$, the lemma is obviously true. So, in what follows we assume that $n \geq 7$. Firstly, we deduce that if $m_1, n_1 \geq 1$ then

$$\begin{aligned}
&ABC_{GG}(S_n^{3,3}(m_1, n_1, m_0)) = \\
&\left(\sqrt{\frac{m_1}{m_1+1}} + \sqrt{\frac{n-m_1-3}{n-m_1-2}} + \sqrt{\frac{n-3}{(m_1+1)(n-m_1-2)}}\right) \\
&+ \left(\sqrt{\frac{n_1}{n_1+1}} + \sqrt{\frac{n-n_1-3}{n-n_1-2}} + \sqrt{\frac{n-3}{(n_1+1)(n-n_1-2)}}\right) \\
&+ (n-5)\sqrt{\frac{n-2}{n-1}}. \qquad (1)
\end{aligned}$$

If $m_1, m_2 > 0$, by Lemma 2.1 we have

$$\sqrt{\frac{m_1+m_2}{(m_1+1)(m_2+1)}} \leq \sqrt{\frac{1}{2}} \leq \sqrt{\frac{m_1}{m_1+1}},$$

$$\sqrt{\frac{n-m_1-3}{(m_2+1)(n-m_1-m_2-2)}} \leq \sqrt{\frac{1}{2}} \leq \sqrt{\frac{n-m_1-3}{n-m_1-2}},$$

$$\sqrt{\frac{n-m_2-3}{(m_1+1)(n-m_1-m_2-2)}} < \sqrt{\frac{n-3}{(m_1+1)(n-m_1-2)}} .$$

These inequalities still hold for $n_1, n_2 > 0$.

When $m_1, m_2, n_1, n_2 > 0$, we have

$$\begin{aligned}
& ABC_{GG}(S_n^{3,3}(m_1, m_2, n_1, n_2, m_0)) \\
= & \sqrt{\frac{m_1+m_2}{(m_1+1)(m_2+1)}} + \sqrt{\frac{n-m_2-3}{(m_1+1)(n-m_1-m_2-2)}} \\
& + \sqrt{\frac{n-m_1-3}{(m_2+1)(n-m_1-m_2-2)}} + \sqrt{\frac{n_1+n_2}{(n_1+1)(n_2+1)}} \\
& + \sqrt{\frac{n-n_2-3}{(n_1+1)(n-n_1-n_2-2)}} + \sqrt{\frac{n-n_1-3}{(n_2+1)(n-n_1-n_2-2)}} \\
& +(n-5)\sqrt{\frac{n-2}{n-1}} \\
< & ABC_{GG}(S_n^{3,3}(m_1, n_1, m_0+m_2+n_2)).
\end{aligned}$$

When exactly one of m_1, m_2, n_1, n_2 equals zero, say, $m_2 = 0$. Hence,

$$\begin{aligned}
& ABC_{GG}(S_n^{3,3}(m_1, 0, n_1, n_2, m_0)) \\
= & \sqrt{\frac{m_1}{m_1+1}} + \sqrt{\frac{n-m_1-3}{n-m_1-2}} + \sqrt{\frac{n-3}{(m_1+1)(n-m_1-2)}} \\
& + \sqrt{\frac{n_1+n_2}{(n_1+1)(n_2+1)}} + \sqrt{\frac{n-n_2-3}{(n_1+1)(n-n_1-n_2-2)}} \\
& + \sqrt{\frac{n-n_1-3}{(n_2+1)(n-n_1-n_2-2)}} + (n-5)\sqrt{\frac{n-2}{n-1}} \\
< & ABC_{GG}(S_n^{3,3}(m_1, n_1, m_0+n_2)).
\end{aligned}$$

When exactly two of m_1, m_2, n_1, n_2 equal zero, if $m_1 = m_2 = 0$ (the case when $n_1 = n_2 = 0$ is similar) then G has unique non-pendent edge uv such that $n_u = n_v = 1$, which contributes 0 to the index; G also has two such non-pendent edges uv and xy that $n_u = 1$ and $n_v = n-2$, each of them contributes $\sqrt{\frac{n_u+n_v-2}{n_un_v}}=\sqrt{\frac{n-3}{n-2}}$ to the index. So,

$$\begin{aligned}
& ABC_{GG}(S_n^{3,3}(0,0,n_1,n_2,m_0)) \\
= \;& 2\sqrt{\frac{n-3}{n-2}}+\sqrt{\frac{n_1+n_2}{(n_1+1)(n_2+1)}}+\sqrt{\frac{n-n_2-3}{(n_1+1)(n-n_1-n_2-2)}} \\
& +\sqrt{\frac{n-n_1-3}{(n_2+1)(n-n_1-n_2-2)}}+(n-5)\sqrt{\frac{n-2}{n-1}} \\
< \;& ABC_{GG}(S_n^{3,3}(m_1,n_1,m_0^{'})).
\end{aligned}$$

Since G has maximal ABC_{GG} index, it follows that $\min\{n_1,n_2\}=0$ and $\min\{m_1,m_2\}=0$. ■

Lemma 3.5. *Let $G\in S_n^{r,t}$ be a connected bicyclic graph with $n\geq 6$.*

(1) If $n=6$ then $ABC_{GG}(G)\leq\sqrt{3}+\sqrt{2}+\sqrt{\frac{2}{3}}+\sqrt{\frac{4}{5}}$, with equality holding if and only if $G=S_6^{3,3}(1,0,0)$.

(2) If $n=7$ then $ABC_{GG}(G)\leq\sqrt{3}+2\sqrt{2}+2\sqrt{\frac{5}{6}}$, with equality holding if and only if $G=S_7^{3,3}(1,1,0)$.

(3) If $n=8$ then $ABC_{GG}(G)\leq\sqrt{2}+\sqrt{\frac{2}{3}}+\sqrt{\frac{3}{4}}+\sqrt{\frac{4}{5}}+\sqrt{\frac{5}{12}}+3\sqrt{\frac{6}{7}}$, with equality holding if and only if $G=S_8^{3,3}(2,1,0)$.

(4) If $n=9$ then $ABC_{GG}(G)\leq 2\sqrt{\frac{2}{3}}+2\sqrt{\frac{6}{15}}+2\sqrt{\frac{4}{5}}+4\sqrt{\frac{7}{8}}$, with equality holding if and only if $G=S_9^{3,3}(2,2,0)$.

(5) If $10\leq n\leq 15$ then $ABC_{GG}(G)\leq 2\left(\sqrt{\frac{2}{3}}+\sqrt{\frac{n-5}{n-4}}+\sqrt{\frac{n-3}{3(n-4)}}\right)+(n-5)\sqrt{\frac{n-2}{n-1}}$, with equality holding if and only if $G=S_n^{3,3}(2,2,n-9)$.

(6) If $n\geq 16$ then $ABC_{GG}(G)\leq 2\left(\sqrt{2}+\sqrt{\frac{n-4}{n-3}}\right)+(n-5)\sqrt{\frac{n-2}{n-1}}$, with equality holding if and only if $G=S_n^{3,3}(1,1,n-7)$.

Proof. Let $G\in S_n^{3,3}$ be a connected bicyclic graph with maximal ABC_{GG} index. If $n=6$, then $G\in\{S_6^{3,4}(0,0,0,0,0),S_6^{3,3}(1,0,0),S_6^{3,3}(0,0,1)\}$. Since

$$ABC_{GG}(S_6^{3,3}(1,0,0))=\sqrt{3}+\sqrt{2}+\sqrt{\frac{2}{3}}+\sqrt{\frac{4}{5}}\approx 4.8572,$$
$$ABC_{GG}(S_6^{3,4}(0,0,0,0,0))=\sqrt{3}+2\sqrt{2}\approx 4.5605,$$

$$ABC_{GG}(S_6^{3,3}(0,0,1)) = 2\sqrt{3} + \sqrt{\frac{4}{5}} \approx 4.3585.$$

It implies that (1) holds.

If $n = 7$, by Lemmas 3.1(1), 3.3, 3.4 and equation (1) we have

$$ABC_{GG}(G) \leq ABC_{GG}(S_7^{3,3}(1,1,0)) = \sqrt{3} + 2\sqrt{2} + 2\sqrt{\frac{5}{6}}$$

with equality holding if and only if $G = S_7^{3,3}(1,1,0)$.

If $n = 8$, by Lemma 3.1(1), (2), Lemmas 3.3, 3.4 and equation (1) we have

$$ABC_{GG}(G) \leq ABC_{GG}(S_8^{3,3}(2,1,0)) = \sqrt{2}+\sqrt{\frac{2}{3}}+\sqrt{\frac{3}{4}}+\sqrt{\frac{4}{5}}+\sqrt{\frac{5}{12}}+3\sqrt{\frac{6}{7}}$$

with equality holding if and only if $G = S_8^{3,3}(2,1,0)$.

If $n = 9$, by Lemma 3.1(1), (2), (3), Lemmas 3.3, 3.4 and equation (1) we have $ABC_{GG}(S_9^{3,3}(3,1,0)) = 2\sqrt{\frac{3}{4}} + \sqrt{\frac{3}{8}} + \sqrt{\frac{4}{5}} + \sqrt{\frac{5}{6}} + 4\sqrt{\frac{7}{8}} \approx 7.8934 < ABC_{GG}(S_9^{3,3}(2,2,0)) = 2\sqrt{\frac{2}{3}} + 2\sqrt{\frac{6}{15}} + 2\sqrt{\frac{4}{5}} + 4\sqrt{\frac{7}{8}} \approx 8.4284$. So,

$$ABC_{GG}(G) \leq ABC_{GG}(S_9^{3,3}(2,2,0)) = 2\sqrt{\frac{2}{3}} + 2\sqrt{\frac{6}{15}} + 2\sqrt{\frac{4}{5}} + 4\sqrt{\frac{7}{8}}$$

with equality holding if and only if $G = S_9^{3,3}(2,2,0)$.

If $10 \leq n \leq 15$, by equation (1) and Lemma 3.1(4), Lemmas 3.3 and 3.4 we have

$$\begin{aligned} ABC_{GG}(G) &\leq ABC_{GG}(S_n^{3,3}(2,2,n-9)) \\ &= 2\left(\sqrt{\frac{2}{3}} + \sqrt{\frac{n-5}{n-4}} + \sqrt{\frac{n-3}{3(n-4)}}\right) + (n-5)\sqrt{\frac{n-2}{n-1}} \end{aligned}$$

with equality holding if and only if $G = S_n^{3,3}(2,2,n-9)$.

Finally, if $n \geq 16$, by equation (1) and Lemma 3.1(5), Lemmas 3.3 and

3.4 we have

$$\begin{aligned} ABC_{GG}(G) &\leq ABC_{GG}(S_n^{3,3}(1,1,n-7)) \\ &= 2\left(\sqrt{2}+\sqrt{\frac{n-4}{n-3}}\right)+(n-5)\sqrt{\frac{n-2}{n-1}} \end{aligned}$$

with equality holding if and only if $G = S_n^{3,3}(1,1,n-7)$. ■

Let $C_4 = v_1v_2v_3v_4v_1$ be a cycle of order 4 and $Q_4 = C_4 + v_1v_3$. Denote by $B_n(n_1, n_2, n_3, n_4)$ be the graph obtained from Q_4 by attaching $n_i - 1 \geq 0$ isolated vertices to v_i for all $i = 1, 2, 3, 4$ with $n_1 \geq n_2 \geq n_3 \geq n_4$. Then $B_{n,n-4}$ is the set of all such graphs $B_n(n_1, n_2, n_3, n_4)$ with $n_1 + n_2 + n_3 + n_4 = 5$.

Lemma 3.6. *Let $G = B_n(n_1, n_2, n_3, n_4)$ be a graph with $n_1, n_2, n_3, n_4 \geq 1$. Then $ABC_{GG}(G) < ABC_{GG}(B_n(n_1 + 1, n_2, n_3 - 1, n_4))$ if $n_2, n_4 \geq 2$ and $n_1 \geq n_3 \geq 2$; $ABC_{GG}(G) < ABC_{GG}(B_n(n_1, n_2 + 1, n_3, n_4 - 1))$ if $n_2 \geq n_4 \geq 2$ and $n_3 = 1$.*

Proof. Since all pendent edges are contribute the same to the ABC_{GG} index, it follows that

$$\begin{aligned} &ABC_{GG}(B_n(n_1+1, n_2, n_3-1, n_4)) - ABC_{GG}(G) \\ &= \left(\sqrt{\frac{n_1+n_2+n_4-1}{(n_1+1+n_4)n_2}} - \sqrt{\frac{n_1+n_2+n_4-2}{(n_1+n_4)n_2}}\right) \\ &- \left(\sqrt{\frac{n_3+n_2+n_4-2}{(n_3+n_4)n_2}} - \sqrt{\frac{n_3+n_2+n_4-3}{(n_3-1+n_4)n_2}}\right) \\ &+ \left(\sqrt{\frac{n_1+n_2+n_4-1}{(n_1+n_2+1)n_4}} - \sqrt{\frac{n_1+n_2+n_4-2}{(n_1+n_2)n_4}}\right) \\ &- \left(\sqrt{\frac{n_2+n_3+n_4-2}{(n_2+n_3)n_4}} - \sqrt{\frac{n_2+n_3+n_4-3}{(n_2+n_3-1)n_4}}\right) \\ &+ \left(\sqrt{\frac{n_1+n_3-2}{(n_1+1)(n_3-1)}} - \sqrt{\frac{n_1+n_3-2}{n_1n_3}}\right). \end{aligned}$$

Since $n_1 \geq n_3 \geq 2$, it follows that

$$\sqrt{\frac{n_1+n_3-2}{(n_1+1)(n_3-1)}} - \sqrt{\frac{n_1+n_3-2}{n_1n_3}} > 0.$$

Recalling that by Lemma 2.2, $g_a(x)$ is strictly increasing for a if $x \geq 3$, and noticing that $g_a(2) = 0$ we deduce that

$$\begin{aligned}
&\left(\sqrt{\frac{n_1+n_2+n_4-1}{(n_1+1+n_4)n_2}} - \sqrt{\frac{n_1+n_2+n_4-2}{(n_1+n_4)n_2}}\right)\\
&-\left(\sqrt{\frac{n_3+n_2+n_4-2}{(n_3+n_4)n_2}} - \sqrt{\frac{n_3+n_2+n_4-3}{(n_3-1+n_4)n_2}}\right)\\
&= g_{n_1+n_4+1}(n_2) - g_{n_3+n_4}(n_2) \geq 0,
\end{aligned}$$

$$\begin{aligned}
&\left(\sqrt{\frac{n_1+n_2+n_4-1}{(n_1+n_2+1)n_4}} - \sqrt{\frac{n_1+n_2+n_4-2}{(n_1+n_2)n_4}}\right)\\
&-\left(\sqrt{\frac{n_2+n_3+n_4-2}{(n_2+n_3)n_4}} - \sqrt{\frac{n_2+n_3+n_4-3}{(n_2+n_3-1)n_4}}\right)\\
&= g_{n_1+n_2+1}(n_4) - g_{n_3+n_2}(n_4) \geq 0.
\end{aligned}$$

Therefore, the first statement is true. For the second one, we have

$$\begin{aligned}
&ABC_{GG}(B_n(n_1, n_2+1, 1, n_4-1)) - ABC_{GG}(B_n(n_1, n_2, 1, n_4))\\
= \quad &\left(\sqrt{\frac{n_1+n_2+n_4-2}{(n_1+n_2+1)(n_4-1)}} - \sqrt{\frac{n_1+n_2+n_4-2}{(n_1+n_2)n_4}}\right)\\
&-\left(\sqrt{\frac{n_1+n_2+n_4-2}{(n_1+n_4)n_2}} - \sqrt{\frac{n_1+n_2+n_4-2}{(n_1+n_4-1)(n_2+1)}}\right)\\
&+\left(\sqrt{\frac{n_2+n_4-1}{(n_2+2)(n_4-1)}} - \sqrt{\frac{n_2+n_4-1}{(n_2+1)n_4}}\right)\\
&+\left(\sqrt{\frac{n_2+n_4-1}{n_4(n_2+1)}} - \sqrt{\frac{n_2+n_4-1}{(n_4+1)n_2}}\right).
\end{aligned}$$

Since $n_2 \geq n_4 \geq 2$, it follows that the first, third term are all positive, and the fourth term is nonnegative. The second term is also positive if $n_2 \geq n_1 + n_4$, and so the second statement is true in this case. In what follows we consider the other case when $n_2 < n_1 + n_4$. It suffices to show that the sum of the first and second term is nonnegative, or

$$\sqrt{\frac{1}{(n_1+n_2+1)(n_4-1)}} - \sqrt{\frac{1}{(n_1+n_2)n_4}} \geq \sqrt{\frac{1}{(n_1+n_4)n_2}} - \sqrt{\frac{1}{(n_1+n_4-1)(n_2+1)}}.$$

Let $m = n_1+n_2+n_4 = n-1$ and $g(x) = \frac{1}{\sqrt{x(m-x)}} - \frac{1}{\sqrt{(x+1)(m-x-1)}}$ with $1 \leq x < \frac{m}{2}$. Then $m \geq 5$, and the above inequality becomes $g(n_4-1) \geq g(n_2)$. So, to show the above inequality we need only show that $g(x)$ is decreasing when $1 \leq x < \frac{m}{2}$. Noticing that

$$\frac{dg}{dx} = \frac{m-2x-2}{2\left((x+1)(m-x-1)\right)^{3/2}} - \frac{m-2x}{2\left(x(m-x)\right)^{3/2}},$$

to show $\frac{dg}{dx} < 0$ it suffices to show that

$$(m-2x)^2(x+1)^3(m-x-1)^3 > x^3(m-x)^3(m-2x-2)^2.$$

But this is obvious since $(x+1)/(m-x) > x/(m-x-1)$ for all x with $1 \leq x < m/2$. And so, the second statement is true. ■

The above Lemma tell us that in $B_{n,n-4}$, graphs with maximal ABC_{GG} index are of the form $B_n(n_1, n_2, 1, 1)$, where $n_1, n_2 \geq 1$.

Lemma 3.7. *If $G = B_n(n_1, n_2, 1, 1)$, then $ABC_{GG}(G) \leq 2\sqrt{\frac{n-3}{n-2}} + \sqrt{2} + \sqrt{\frac{n-4}{n-3}} + (n-4)\sqrt{\frac{n-2}{n-1}}$, with the equality holding if and only if $G = B_n(n-3, 1, 1, 1)$.*

Proof. Since

$$ABC_{GG}(G) = \sqrt{\frac{n-3}{(n_1+1)n_2}} + \sqrt{\frac{n_2}{n_2+1}} + \sqrt{\frac{n_1-1}{n_1}} + \sqrt{\frac{n-3}{n-2}}$$

$$+\sqrt{\frac{1}{2}}+(n-4)\sqrt{\frac{n-2}{n-1}},$$

$$\begin{aligned} ABC_{GG}(B_n(n-3,1,1,1)) &= 2\sqrt{\frac{n-3}{n-2}}+\sqrt{\frac{n-4}{n-3}}+\sqrt{2} \\ &\quad +(n-4)\sqrt{\frac{n-2}{n-1}}. \end{aligned}$$

we have

$$\begin{aligned} &ABC_{GG}(B_n(n-3,1,1,1)) - ABC_{GG}(G) \\ &= \left(\sqrt{\frac{n-3}{n-2}}-\sqrt{\frac{n_2}{n_2+1}}\right)+\left(\sqrt{\frac{1}{2}}-\sqrt{\frac{n-3}{(n_1+1)n_2}}\right) \\ &+\left(\sqrt{\frac{n-4}{n-3}}-\sqrt{\frac{n_1-1}{n_1}}\right). \end{aligned}$$

If $n_1, n_2 \geq 2$, then $n_1, n_2 \leq n-4$. And so, $ABC_{GG}(G) < ABC_{GG}(B_n(n-3,1,1,1))$. This observation shows that $ABC_{GG}(G) = ABC_{GG}(B_n(n-3,1,1,1))$ only if $n_1 = 1$ or $n_2 = 1$. By direct calculation the above difference one can show that $n_2 = 1$. And so, the lemma follows. ■

Let $B_n^{r,t}(s)$ be the set of all such n-vertex bicyclic graphs whose two cycles C_r and C_t have shortest common path P_s, and every vertex not in these two cycles is pendent, where $s \geq 2$ and $r \geq t \geq 3$.

Lemma 3.8. *Let G be a connected bicyclic graph of order $n \geq 5$, whose two cycles C_r and C_t have shortest common path P_s with $s \geq 2$ and $r \geq t \geq 3$. Then $ABC_{GG}(G) < ABC_{GG}(B_n(n-3,1,1,1))$.*

Proof. Assume that G has maximal ABC_{GG} index in all the graphs postulated in this lemma. By the Lemma 3.2, $G \in B_n^{r,t}(s)$.

If $s \geq 3$, then $r \geq t \geq 4$, $t-s \geq 1$ and $r+t-s \geq 2+s \geq 5$. In this case, $n_u, n_v \geq 2$ for each $uv \in E(C_r) \cup E(C_t)$. And so,

$$\sqrt{\frac{n_u+n_v-2}{n_u n_v}} \leq \sqrt{\frac{1}{2}} < \sqrt{\frac{n-2}{n-1}}.$$

Hence,

$$\begin{aligned}
ABC_{GG}(G) &= \sum_{\substack{uv\in E(G)\\ d_u=1}} \sqrt{\frac{n_u+n_v-2}{n_un_v}} + \sum_{\substack{uv\in E(G)\\ d_u,d_v\neq 1}} \sqrt{\frac{n_u+n_v-2}{n_un_v}} \\
&\leq (n-r-t+s)\sqrt{\frac{n-2}{n-1}} + (r+t-s+1)\sqrt{\frac{1}{2}} \\
&= (n-4)\sqrt{\frac{n-2}{n-1}} + (s-r-t+4)\sqrt{\frac{n-2}{n-1}} \\
&\quad +(r+t-s-4)\sqrt{\frac{1}{2}} + 5\sqrt{\frac{1}{2}} \\
&< (n-4)\sqrt{\frac{n-2}{n-1}} + 5\sqrt{\frac{1}{2}} \\
&< 2\sqrt{\frac{n-3}{n-2}} + \sqrt{2} + \sqrt{\frac{n-4}{n-3}} + (n-4)\sqrt{\frac{n-2}{n-1}} \\
&= ABC_{GG}(B_n(n-3,1,1,1)).
\end{aligned}$$

If $s=2$ and $r,t\geq 4$, then the above inequalities are also true. Finally, we consider the case when $s=2$ and $r\geq 4$, $t=3$. Assume the number of pendent vertices adjacent to the vertex of C_t-C_r is m. Noticing that $n\geq 5$ in this case, we have

$$ABC_{GG}(G) \leq r\sqrt{\tfrac{1}{2}} + (n-r-1)\sqrt{\tfrac{n-2}{n-1}} + \begin{cases} 2\sqrt{\frac{1}{2}}, & \text{if } m\geq 1; \\ 2\sqrt{\frac{n-4}{n-3}}, & \text{if } m=0. \end{cases}$$

$$< r\sqrt{\tfrac{1}{2}} + (3-r)\sqrt{\tfrac{n-2}{n-1}} + (n-4)\sqrt{\tfrac{n-2}{n-1}} + \begin{cases} 2\sqrt{\frac{1}{2}}, & \text{if } m\geq 1; \\ 2\sqrt{\frac{n-4}{n-3}}, & \text{if } m=0. \end{cases}$$

$$< 3\sqrt{\tfrac{1}{2}} + (n-4)\sqrt{\tfrac{n-2}{n-1}} + \begin{cases} 2\sqrt{\frac{1}{2}}, & \text{if } m\geq 1; \\ 2\sqrt{\frac{n-4}{n-3}}, & \text{if } m=0. \end{cases}$$

$$< ABC_{GG}(B_n(n-3,1,1,1)).$$

The above discussion shows that $G=B_n(n_1,n_2,n_3,n_4)$. And so, the lemma follows from Lemmas 3.6 and 3.7. ■

Theorem 3.1. *If G is a connected bicyclic graph of order $n\geq 4$ then $ABC_{GG}(G)\leq 2\sqrt{\frac{n-3}{n-2}}+\sqrt{2}+\sqrt{\frac{n-4}{n-3}}+(n-4)\sqrt{\frac{n-2}{n-1}}$, with equality holding if and only if $G=B_n(n-3,1,1,1)$.*

Proof. The case when $n = 4$ is trivial. Suppose in what follows that $n \geq 5$. If $n = 5$, by the Lemmas 3.6, 3.7 and 3.8, we need only to compare $ABC_{GG}(B_5(2,1,1,1))$ and $ABC_{GG}(S_5^{3,3}(0,0,0)$. Since $ABC_{GG}(B_5(2,1,1,1)) = 2\sqrt{\frac{2}{3}}+3\sqrt{\frac{1}{2}}+\sqrt{\frac{3}{4}} > 4\sqrt{\frac{2}{3}} = ABC_{GG}(S_5^{3,3}(0,0,0))$, the theorem follows in this case. Theorem is also true when $n = 6$ since $ABC_{GG}(B_6(3,1,1,1)) = \sqrt{3}+\sqrt{2}+\sqrt{\frac{2}{3}}+2\sqrt{\frac{4}{5}} > \sqrt{2}+\sqrt{3}+\sqrt{\frac{2}{3}}+\sqrt{\frac{4}{5}} = ABC_{GG}(S_6^{3,3}(1,0,0))$.

When $n = 7$, $ABC_{GG}(B_7(4,1,1,1)) = 2\sqrt{\frac{4}{5}} + \sqrt{2} + \sqrt{\frac{3}{4}} + 3\sqrt{\frac{5}{6}} \approx 6.8077$ and $ABC_{GG}(S_7^{3,3}(1,1,0)) = \sqrt{3} + 2\sqrt{2} + 2\sqrt{\frac{5}{6}} \approx 6.3862$; When $n = 8$, $ABC_{GG}(B_8(5,1,1,1)) = 2\sqrt{\frac{5}{6}} + \sqrt{2} + \sqrt{\frac{4}{5}} + 4\sqrt{\frac{6}{7}} \approx 7.8377$ and $ABC_{GG}(S_8^{3,3}(2,1,0)) = \sqrt{\frac{2}{3}} + \sqrt{\frac{3}{4}} + \sqrt{\frac{4}{5}} + \sqrt{\frac{5}{12}} + \sqrt{2} + 3\sqrt{\frac{6}{7}} \approx 7.4141$; When $n = 9$, $ABC_{GG}(B_9(6,1,1,1)) = 2\sqrt{\frac{6}{7}} + \sqrt{2} + \sqrt{\frac{5}{6}} + 5\sqrt{\frac{7}{8}} \approx 8.8558$ and $ABC_{GG}(S_9^{3,3}(2,2,0)) = 2\sqrt{\frac{2}{3}} + 2\sqrt{\frac{6}{15}} + 2\sqrt{\frac{4}{5}} + 4\sqrt{\frac{7}{8}} \approx 8.4284$. And so, the theorem is also true in all these cases.

If $10 \leq n \leq 15$, by Lemmas 3.5, 3.6, 3.7 and 3.8, we need only to compare $ABC_{GG}(B_n(n-3,1,1,1)) = 2\sqrt{\frac{n-3}{n-2}}+\sqrt{2}+\sqrt{\frac{n-4}{n-3}}+(n-4)\sqrt{\frac{n-2}{n-1}}$ and $ABC_{GG}(S_n^{3,3}(2,2,n-9)) = 2\left(\sqrt{\frac{2}{3}} + \sqrt{\frac{n-5}{n-4}} + \sqrt{\frac{n-3}{3(n-4)}}\right) + (n-5)\sqrt{\frac{n-2}{n-1}}$. Since $n-1 > n-3 > n-4$, by Lemma 2.1 we conclude that $ABC_{GG}(B_n(n-3,1,1,1)) - ABC_{GG}(S_n^{3,3}(2,2,n-9)) = 2\sqrt{\frac{n-3}{n-2}} - 2\sqrt{\frac{2}{3}} + \sqrt{2} - 2\sqrt{\frac{n-3}{3(n-4)}} + \sqrt{\frac{n-4}{n-3}} - \sqrt{\frac{n-5}{n-4}} + \sqrt{\frac{n-2}{n-1}} - \sqrt{\frac{n-5}{n-4}} > 0$. Hence,

$$ABC_{GG}(S_n^{3,3}(2,2,n-9)) < ABC_{GG}(B_n(n-3,1,1,1)).$$

Finally, if $n \geq 16$, since $ABC_{GG}(S_n^{3,3}(1,1,n-7)) = 2\left(\sqrt{2} + \sqrt{\frac{n-4}{n-3}}\right) + (n-5)\sqrt{\frac{n-2}{n-1}}$ it follows that $ABC_{GG}(B_n(n-3,1,1,1)) - ABC_{GG}(S_n^{3,3}(1,1,n-7)) = 2\sqrt{\frac{n-3}{n-2}} - \sqrt{2} + \sqrt{\frac{n-2}{n-1}} - \sqrt{\frac{n-4}{n-3}} > 0$. Hence,

$$ABC_{GG}(S_n^{3,3}(1,1,n-7)) < ABC_{GG}(B_n(n-3,1,1,1)).$$

By Lemmas 3.5, 3.6, 3.7 and 3.8, the theorem follows. ■

***Acknowledgment*:** This work is supported by the National Natural Science Foundation of China (grant number 12061074, 12201471), the Doctoral Research Foundation of Longdong University (XYBYZK2306, XYBYZK2307), the Special Foundation in Key Fields for Universities of Guangdong Province (2022ZDZX1034).

References

[1] S. J. Cyvin, I. Gutman, *Kekule Structures in Benzenoid Hydrocarbons, Lecture Notes in Chemistry*, Springer–Verlag, Berlin, 1988.

[2] K. C. Das, I. Gutman, B. Furtula, On atom-bond connectivity index, *Chem. Phys. Lett.* **511** (2011) 452–454.

[3] K. C. Das, I. Gutman, B. Furtula, On atom-bond connectivity index, *Filomat* **26** (2012) 733–738.

[4] K. C. Das, N. Trinajstić, Comparison between first geometric-arithmetic index and atom-bond connectivity index, *Chem. Phys. Lett.* **497** (2010) 149–151.

[5] K. C. Das, K. Xu, A. Graovac, Maximal unicyclic graphs with respect to new atom-bond connectivity index, *Acta Chim. Slov.* **60** (2013) 34–42.

[6] J. Devillers, A. T. Balaban (Eds.), *Topological indices and related descriptors in QSAR and QSPR*, Gordon & Breach, Amsterdam, 1999.

[7] E. Estrada, Atom-bond connectivity and the energetic of branched alkanes, *Chem. Phys. Lett.* **463** (2008) 422–425.

[8] E. Estrada, L. Torres, L. Rodriguez, I. Gutman, An atom-bond connectivity index: Modeling the enthalpy of formation of alkanes, *Indian J.Chem.* **37A** (1998) 849–855.

[9] G. H. Fath-Tabar, B. Vaez-Zadeh, A. R. Ashrafi, A. Graovac, Some inequalities for the atom-bond connectivity index of graph operations, *Discrete Applied Math.* **159** (2011) 1323–1330.

[10] S. Filipovski, Connected graphs with maximal Graovac-Ghorbani index, *MATCH Commun. Math. Comput. Chem.* **89** (2023) 517–525.

[11] B. Furtula, Atom-bond connectivity index versus Graovac-Ghorbani analog, *MATCH Commun. Math. Comput. Chem.* **75** (2016) 233–242.

[12] B. Furtula, A. Graovac, D. Vukičević, Atom-bond connectivity index of trees, *Discr. Applied Math.* **157** (2009) 2828–2835.

[13] W. Gao, W. Wang, Second atom-bond connectivity index of special chemical molecular structures, *J. Chem.* (2014) #906254.

[14] A. Graovac, M. Ghorbani, A new version of atom-bond connectivity index, *Acta Chim. Slov.* **57** (2010) 609–612.

[15] A. Graovac, I. Gutman, N. Trinajstić, *Topological Approach to the Chemistry of Conjugated Molecules*, Springer–Verlag, Berlin, 1977.

[16] I. Gutman, B. Furtula, M. Ivanović, Notes on trees with minimal atom-bond connectivity index, *MATCH Commun. Math. Comput. Chem.* **67** (2012) 467–482.

[17] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer–Verlag, Berlin, 1986.

[18] D. Pacheco, L. de Lima, C. S. Oliveira, On the Graovac-Ghorbani Index for Bicyclic Graph with No Pendent Vertices, *MATCH Commun. Math. Comput. Chem.* **86** (2021) 429–448.

[19] M. Randić, On characterization of molecular branching, *J. Amer. Chem. Soc.* **97** (1975) 6609–6615.

[20] M. Rostami, M. Sohrabi-Haghighat, Further results on new version of atom-bond connectivity index, *MATCH Commun. Math. Comput. Chem.* **71** (2014) 21–32.

[21] Z. Tang, Y. Hou, Note on the second atom-bond connectivity index, *Journal of Natural Science of Hunan Normal University*, **38** (2015) 80–84.

[22] N. Trinajstić, I. Gutman, Mathematical chemistry, *Croat. Chem. Acta.* **75** (2002) 329–356.

[23] R. Xing, B. Zhou, F. Dong, On atom-bond connectivity index of connected graphs, *Discrete Applied Math.* **159** (2011) 1617–1630.

[24] R. Xing, B. Zhou, Z. Du, Further results on atom-bond connectivity index of trees, *Discrete Applied Math.* **158** (2010) 1536–1545.

[25] B. Zhou, R. Xing, On atom-bond connectivity index, *F. Naturforsch.* **A66** (2011) 61–66.