Short Communication

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On the maximum *ABC* index of bipartite graphs without pendent vertices
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Abstract: For a simple graph G , the atom–bond connectivity index (*ABC*) of G is defined as $ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}$, where $d(v)$ denotes the degree of vertex v of G . In this paper, we prove that for any bipartite graph G of order $n \geq 6$, size $2n - 3$ with $\delta(G) \geq 2$, $ABC(G) \leq \sqrt{2}(n - 6) + 2\sqrt{\frac{3(n-2)}{n-3}} + 2$, and we characterize all extreme bipartite graphs.

Keywords: degree (of vertex); atom–bond connectivity index; bipartite graph; extremal graph; incidence energy.

1 Introduction

Let G be a simple connected graph with vertex set $V = V(G)$ and edge set $E = E(G)$, in which a simple graph contains no loops and duplicate edges between two vertices. The order $|V|$ of G is denoted by $n = n(G)$, and the size $|E|$ of G is denoted by $m = m(G)$. For every vertex $v \in V$, the *open neighborhood* $N(v)$ is the set $\{u \in V(G) \mid uv \in E(G)\}$. The *degree* of a vertex $v \in V$ is $d_G(v) = d(v) = |N(v)|$. The *minimum degree* of a graph G are denoted by $\delta = \delta(G)$. A *leaf* or a *pendant vertex* of a graph G is a vertex of degree 1. For a subset S of vertices of G , we denote by $G[S]$ the subgraph induced by S . A bipartite graph is a graph having no odd cycles.

The connectivity index, χ , is a topological index introduced in 1975 by Milan Randić [1] who has shown this index to reflect molecular branching. However, many physico-chemical properties are dependent on factors rather different than branching. In order to take this into account along with keeping the spirit of the Randić in-

dex, Ernesto Estrada *et al.* [2] proposed a new topological index, named the atom-bond connectivity (*ABC*) index. Estrada [3] proved that the *ABC* index provides a good model for the stability of linear and branched alkanes as well as the strain energy of cycloalkanes. For those who may not be familiar with alkanes, these are any of the series of saturated hydrocarbons having the general formula C_nH_{2n+2} , including methane, ethane and propane. Additional physico-chemical applicabilities of the *ABC* index were presented in a few other works, including [3–5]. The atom-bond connectivity index of G is defined as

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}}. \quad (1)$$

Due to its physico-chemical applicability, the *ABC* index has attracted significant attention from researchers in recent years, and many mathematical properties of this index have been reported [5–15].

When examining a topological index, one of the fundamental questions that needs to be answered is for which graphs this index assumes minimal and maximal values. In addition, the identities of these extremal values must be uncovered. The minimal value of the *ABC* index has been investigated by several authors [16–22], and the maximal value of the *ABC* index has been studied extensively, as well [23–26]. Recently, Shao *et al.* [15, 27] showed that for any connected graph G of order n , size $2n - 4 \geq 4$ with $\delta(G) \geq 2$, $ABC(G) \leq (n - 2)\sqrt{2}$ characterizes all extremal graphs. They also proved that for any connected graph G of order n , size $2n - 3 \geq 5$ with $\delta(G) \geq 2$, characterizes all extremal $(n, 2n - 2)$ graphs without pendent vertices and with maximum *ABC* indices.

In this paper, we focus on bipartite graphs and show that for any bipartite graph G of order n , size $2n - 3$ with $\delta(G) \geq 2$, $ABC(G) \leq \sqrt{2}(n - 6) + 2\sqrt{\frac{3(n-2)}{n-3}} + 2$. We also classify all extreme bipartite graphs.

We make use of the following results and notations in this paper. To simplify notations, we define the following functions:

- $f(x, y) = \sqrt{\frac{x+y-2}{xy}}$,
- $h(x, y) = f(x, y) - f(x + 1, y)$.

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Lemma 1. ([28]) If (x, y) is strictly decreasing for x if $y \geq 3$.

Lemma 2. ([15]) If G is a graph with $\delta(G) \geq 2$ and $xy \in E(G)$, then $f(x, y) \leq \frac{\sqrt{2}}{2}$ with equality if and only if $d(x) = 2$ or $d(y) = 2$ (or both).

The proof of the next result is straightforward and therefore omitted.

Lemma 3. ([28]) For $x, y \geq 2$, if $h_x(x, y) = \frac{\partial f(x, y)}{\partial x}$ and $h_y(x, y) = \frac{\partial f(x, y)}{\partial y}$, then $h_x(x, y) < 0$.

Similarly, we can see that $h_y(x, y) > 0$.

Let $K_{3,t}$ be the complete bipartite graph with bipartite sets $X = \{x_1, x_2, x_3\}$ and $Y = \{y_1, \dots, y_t\}$. For $s \geq 6$, assume $H_s^{3,t}$ is the bipartite graph obtained from $K_{3,t}$ by adding s vertices $v_1, \dots, v_s$ and joining them to x_1 and x_3 (see Figure 1). If $s = 0$, we define $H_s^{3,t}$ to be the graph $K_{3,t}$. The proof of next result is easy to verify by direct calculation.

Observation 4. If $n \geq 6$, then $ABC(H_{n-6}^{3,3}) = \sqrt{2}(n-6) + 2\sqrt{\frac{3(n-2)}{n-3}} + 2$.

In the rest of paper, we employ the following notation defined in [15].

$$V_i^G = \{v \in V(G) | d(v) = i\}, \quad (2)$$

$$V_{3^+}^G = \{v \in V(G) | d(v) \geq 3\} \text{ and } pk = |V_{3^+}^G|, \quad (3)$$

$$E_{s,t}^G = \{uv \in E(G) | d(u) = s \text{ and } d(v) = t\}, \quad (4)$$

$$E_{s,t^+}^G = \{uv \in E(G) | d(u) = s \text{ and } d(v) \geq t\}, \quad (5)$$

$$E_{s^+,t^+}^G = \{uv \in E(G) | d(u) \geq s \text{ and } d(v) \geq t\} \quad (6)$$

and

$$E_V^G = \{uv | uv \in E(G)\}. \quad (7)$$

In the following, we will omit the superscript where no confusion can arise.

For an edge $e = uv \in E(G)$, we define $ABC(e|G) = \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}$. When no confusion can arise, we simplify $ABC(e|G)$ to $ABC(e)$.

2 Main results

In this section, we present an upper bound on the ABC index of a bipartite graph and characterize all extreme bipartite graphs. For any bipartite graph G , we let (X_G, Y_G) denote its bipartition.

Figure 1: (a) the graph $H_3^{3,3}$; (b) the graph $H_s^{3,3}$.

Theorem 5. Let G be a bipartite graph of order $n \geq 6$, size $2n-3$ with $\delta(G) \geq 2$. Then $ABC(G) \leq \sqrt{2}(n-6) + 2\sqrt{\frac{3(n-2)}{n-3}} + 2$ with equality if and only if $G \cong H_{n-6}^{3,3}$.

Proof: We first perform the following steps:

Step 1: Using the software *geng* in package *nauty* [29], we generate the set of all graphs of order $n \in \{6, 7, 8, 9\}$, size $2n-3$ with $\delta(G) \geq 2$.

Step 2: For each graph G in the obtained graphs, we compute $ABC(G)$ according to formula (1). It turns out that the result holds for each $n \in \{6, 7, 8, 9\}$.

Now, assume that $n \geq 10$. Let G_n be the family of graphs G of order n , size $2n-3$, minimum degree $\delta(G) \geq 2$, the maximum ABC index and different from $H_{n-6}^{3,3}$. We will show that $G_n = \emptyset$. Suppose, to the contrary, that $G_n \neq \emptyset$ for some $n \geq 10$. We further assume that n is as small as possible such that $G_n \neq \emptyset$. Let $G \in G_n$. We proceed with establishing several claims.

Claim 1. $k \geq 6$, $|E_{2,2}| = 0$ and $2k-3 = |E_{3^+,3^+}|$.

Proof of Claim 1. Since every edge is incident with two vertices, an edge contributes 2 to the sum of the degrees of the vertices and so

$$\sum_{v \in V_2} d(v) + \sum_{v \in V_{3^+}} d(v) = 2m(G) = 4n-6. \quad (8)$$

Since $|V_3^+| = k$, we have

$$\sum_{v \in V_2} d(v) = 2|V_2| = 2(n-k). \quad (9)$$

Combining (8) and (9), we obtain

$$\sum_{v \in V_{3^+}} d(v) = 2n + 2k - 6. \quad (10)$$

Since

$$\sum_{v \in V_{3^+}} d(v) = 2|E_{3^+,3^+}| + |E_{2,3^+}| \quad (11)$$

and $m(G) = 2n - 3 = |E_{2,2}| + |E_{2,3^+}| + |E_{3^+,3^+}|$, we conclude from (10) that

$$|E_{3^+,3^+}| - |E_{2,2}| = 2k - 3, \quad (12)$$

and so

$$|E_{3^+,3^+}| \geq 2k - 3. \quad (13)$$

Suppose $x = |X_G \cap V_{3^+}|$. Then $k - x = |Y_G \cap V_{3^+}|$ and we have

$$|E_{3^+,3^+}| \leq x(k - x) \leq \frac{k^2}{4}. \quad (14)$$

By (13) and (14), we have $k^2 - 8k + 12 \geq 0$, and this implies that $k \leq 2$ or $k \geq 6$. If $k = 0$, then (11) and (12) imply that $|E_{3^+,3^+}| = |E_{2,3^+}| = 0$ and $|E_{2,2}| = 3$ yielding $G \cong C_3$, which is a contradiction. If $k = 1$, then we deduce from (14) and (12) that $|E_{3^+,3^+}| = 0$ and $|E_{2,2}| = 1$. Let $E_{2,2} = \{uv\}$ and $V_{3^+} = \{w\}$. Since $d(u) = d(v) = 2$ and $|E_{2,2}| = 1$, we must have $uw \in E$, $vw \in E$, which leads to a contradiction. If $k = 2$, then (14) and (12) imply that $|E_{3^+,3^+}| = 1$ and $|E_{2,2}| = 0$. It follows that any vertex of V_2 along with two vertices in V_{3^+} forms a triangular in G , which is a contradiction. Therefore,

$$k \geq 6. \quad (15)$$

Now, we show that $|E_{2,2}| = 0$. Suppose, to the contrary, that $|E_{2,2}| \geq 1$ and let $uv \in E_{2,2}$. Since $k \geq 6$, it follows from (12) that there exists an edge $ts \in E_{3^+,3^+}$ such that $\{s, t\} \cap \{u, v\} = \emptyset$. Assume, with out loss of generality, that $u, t \in X$ and $v, s \in Y$. We consider two cases.

Case 1. $u \notin N(s)$ and $v \notin N(t)$.

Let G' be the graph obtained from G by removing two edges uv, st and adding the edges us, tv . Clearly, G' is a bipartite graph of order n , size $2n - 3$ with $\delta(G') \geq 2$. By Lemma 2, we have

$$\begin{aligned} ABC(G') - ABC(G) &= ABC(us|G') + ABC(tv|G') \\ &\quad - ABC(uv|G) - ABC(ts|G) \\ &= \sqrt{\frac{d(u|G') + d(s|G') - 2}{d(u|G')d(s|G')}} \\ &\quad + \sqrt{\frac{d(t|G') + d(v|G') - 2}{d(t|G')d(v|G')}} \\ &\quad - \sqrt{\frac{d(u|G) + d(v|G) - 2}{d(u|G)d(v|G)}} \end{aligned}$$

$$\begin{aligned} &= \sqrt{\frac{d(t|G) + d(s|G) - 2}{d(t|G)d(s|G)}} \\ &\geq \frac{\sqrt{2}}{2} + \frac{\sqrt{2}}{2} - \frac{\sqrt{2}}{2} - \frac{2}{3} \\ &> 0, \end{aligned}$$

which is a contradiction.

Case 2. $u \in N(s)$ (the case $v \in N(t)$ is similar).

We distinguish two subcases.

Subcase 2.1. $V_2 \cap N(v) \neq \emptyset$.

Let $w \in V_2 \cap N(v)$. Since $k \geq 6$, $|E_{3^+,3^+}| \geq 2k - 3$ and $|E_s \cap E_{3^+,3^+}| \leq k - 1$, there exists an edge $pq \in E_{3^+,3^+}$ such that $s \notin \{p, q\}$. Assume without loss of generality that $p \in X_G$ and $q \in Y_G$. We deduce from $d(u) = d(v) = 2$, $N(u) = \{v, s\}$ and $N(v) = \{u, w\}$ that $u \notin N(q)$ and $p \notin N(v)$. Now, as Case 1, we obtain a contradiction.

Subcase 2.2. $V_2 \cap N(v) = \emptyset$.

Assume that $w \in V_{3^+} \cap N(v)$. Since $k \geq 6$, $|E_{3^+,3^+}| \geq 2k - 3$ and $|E_s \cap E_{3^+,3^+}| + |E_w \cap E_{3^+,3^+}| \leq k$, we conclude that there exists an edge $pq \in E_{3^+,3^+}$ such that $\{p, q\} \cap \{s, w\} = \emptyset$. Assume without loss of generality that $p \in X_G$ and $q \in Y_G$. Since $d(u) = d(v) = 2$, $N(u) = \{v, s\}$ and $N(v) = \{u, w\}$, we have $u \notin N(q)$ and $v \notin N(p)$. As in Case 1, we obtain a contradiction again.

Thus $|E_{2,2}| = 0$ and by (12) we have $|E_{3^+,3^+}| = 2k - 3$. This completes the proof of Claim 1. $\square$

Claim 2. $|E_{2,3}| = 0$.

Proof of Claim 2. Suppose, to the contrary, that $E_{2,3} \neq \emptyset$ and let $uv \in E_{2,3}$. Assume without loss of generality that $d(v) = 2$ and $d(u) = 3$. Since $E_{2,2} = \emptyset$, the other neighbor of v , say t , is in V_{3^+} . We distinguish the following cases.

(2.a). $N(u) \cap V_{3^+} \neq \emptyset$.

Let $w \in N(u) \cap V_{3^+}$ and let $G' = G - v$. Clearly, G' is a bipartite graph of order $n(G') = n - 1$, size $m(G') = (2n - 3) - 2 = 2(n - 1) - 3$ and $\delta(G') \geq 2$. By the choice of n , we have $ABC(G') \leq \sqrt{2}(n - 7) + 2\sqrt{\frac{3(n-3)}{n-4}} + 2$. We also have $ABC(uw|G') = \frac{\sqrt{2}}{2}$, $ABC(uv|G) = ABC(vt|G) = \frac{\sqrt{2}}{2}$ and $ABC(uw|G) = \sqrt{\frac{d(w)+1}{3d(w)}}$. Using inequality

$$2\sqrt{\frac{3(n-3)}{n-4}} - 2\sqrt{\frac{3(n-2)}{n-3}} < \frac{\sqrt{2}}{2} - \frac{2}{3},$$

we obtain

$$\begin{aligned} ABC(G) &\leq ABC(G') - ABC(uw|G') \\ &\quad + ABC(uw|G) + ABC(uv|G) + ABC(vt|G) \end{aligned}$$

$$\begin{aligned}
&\leq \sqrt{2}(n-7) + 2\sqrt{\frac{3(n-3)}{n-4}} + 2 - \frac{\sqrt{2}}{2} + \frac{2}{3} + \frac{\sqrt{2}}{2} \\
&+ \frac{\sqrt{2}}{2} = \sqrt{2}(n-6) + 2 + 2\sqrt{\frac{3(n-3)}{n-4}} - \frac{\sqrt{2}}{2} + \frac{2}{3} \\
&< \sqrt{2}(n-6) + 2 + 2\sqrt{\frac{3(n-2)}{n-3}} = ABC(H_{n-6}^{3,3}),
\end{aligned}$$

which is a contradiction.

(2.b). $N(u) \cap V_{3^+} = \emptyset$.

Since $|E_{3^+,3^+}| = 2k - 3 \geq 9$, there is an edge $sh \in E_{3^+,3^+}$. Assume without loss of generality that $u, s \in Y$ and $v, h \in X$. First let $s \notin N(v)$. Suppose G' is the graph obtained from G by removing the edges vu, sh and adding the edges vs and uh . Clearly, G' is bipartite of order n , size $2n - 3$ and $\delta(G') \geq 2$. Since $ABC(uh|G') \geq ABC(sh|G)$ and $ABC(vs|G') = ABC(vu|G)$, we have $ABC(G') \geq ABC(G)$ yielding $ABC(G') = ABC(G)$. Hence, $G' \in G_n$. By Claim 1, we have $k \geq 6$, $|E_{2,2}^{G'}| = 0$ and $2k - 3 = |E_{3^+,3^+}^{G'}|$. If $w \in N_G(u) - \{v\}$, then by assumption we have $uw \in E_{2,3}^{G'} \cap E_u^{G'}$. Considering the edge $uw \in G'$, we are in situation (a) and we obtain a contradiction.

Now let $s \in N(v)$. Using an argument similar to that described in Case 2 of Claim 1, we deduce that there exists an edge $pq \in E_{3^+,3^+}$ such that $s \notin \{p, q\}$. Using the proof of Case (b), we obtain a contradiction again.

This completes the proof of Claim 2. $\square$

Claim 3. There exists a bipartite graph $G' = (X_{G'}, Y_{G'})$ of order n , size $2n - 3$ and $\delta(G') \geq 2$, which satisfies the following conditions:

- (i) $ABC(G') \geq ABC(G)$,
- (ii) $|\bigcup_{u \in V_2^{G'} \cap X_{G'}} N(u)| = 2$ or $V_2^{G'} \cap X_{G'} = \emptyset$,
- (iii) $|\bigcup_{u \in V_2^{G'} \cap Y_{G'}} N(u)| = 2$ or $V_2^{G'} \cap Y_{G'} = \emptyset$.

Proof of Claim 3. For any bipartite graph G_1 of order n , size $2n - 3$ and $\delta(G_1) \geq 2$, we define and $L(G_1) = |A(G_1)|$. Let H be the family of bipartite graphs $H \neq H_{n-6}^{3,3}$ such that $|V(H)| = n$, $m(H) = 2n - 3$, $\delta(H) \geq 2$ and $ABC(H) \geq ABC(G)$. Since $G \in H$, we establish that $H \neq \emptyset$. Choose a graph $G' \in H$ such that $L(G')$ is as small as possible. Clearly, G' satisfies in the condition (i). Then $G' \in G_n$ and so G' satisfies Claims 1 and 2. If G' satisfies in the conditions (ii) and (iii) of Claim 3, then we are done. Assume that G' does not satisfy in the condition (ii) or (iii). Assume without loss of generality that G' does not satisfy condition (ii). Then $|V_2^{G'} \cap X_{G'}| \notin \{0, 1\}$. It follows that $|\bigcup_{u \in V_2^{G'} \cap X_{G'}} N(u)| \geq 3$. Then there are two vertices $u_1, u_2 \in V_2^{G'} \cap X_{G'}$ such that $N_{G'}(u_1) \neq N_{G'}(u_2)$. Let $N_{G'}(u_1) = \{v_1, v_2\}$. Since $E_{2,2}^{G'} = \emptyset$, we have $d(v_1|G') \geq 3$ and $d(v_2|G') \geq 3$. We consider the following cases.

Case A. $|N_{G'}(u_1) \cap N_{G'}(u_2)| = 1$.

Suppose without loss of generality that $N_{G'}(u_2) = \{v_2, v_3\}$ and that $d(v_1|G') \leq d(v_3|G')$. Let

$$\begin{aligned}
U_1 &= \{v \in V_2^{G'} \cap X_{G'} | N_{G'}(v) = \{v_1, v_2\}\} \\
&= \{a_1 (= u_1), \dots, a_{k_1}\},
\end{aligned}$$

$$\begin{aligned}
U_2 &= \{v \in V_3^{G'} | v_3 \in N_{G'}(v) \text{ and } v_1 \notin N_{G'}(v)\} \\
&= \{b_1, b_2, \dots, b_{k_2}\},
\end{aligned}$$

and $|U_1| = k_1$, $|U_2| = k_2$. Clearly, $k_1 \geq 1$, $k_2 \geq 0$. We distinguish the following sub-cases.

Subcase A.1. $k_2 \geq k_1$.

Let G_s be the graph obtained from G' by removing the edges v_1a_i, v_3b_i ($1 \leq i \leq k_1$) and adding the edges v_3a_i, v_1b_i ($1 \leq i \leq k_1$). Clearly, G_s is bipartite, and $ABC(a_iv_1|G') = ABC(a_iv_3|G_s)$ for $1 \leq i \leq k_1$. Since $d(v_1|G') \leq d(v_3|G')$, we have $d(v_1|G_s) \leq d(v_3|G_s)$, and this implies that $ABC(b_iv_3|G') \leq ABC(b_iv_1|G_s)$ for $1 \leq i \leq k_1$. Hence $ABC(G_s) \geq ABC(G')$. By definition of $H_{n-6}^{3,3}$, we have $G_s \neq H_{n-6}^{3,3}$ and so $G_s \in H$. This contradicts the choice of G' since $L(G_s) = L(G') - 1$.

Subcase A.2. $k_2 = 0$ and $d(v_1|G') \leq k_1 + 1$.

In this case we have $1 \leq d(v_1|G') - 2 \leq k_1 - 1$. Let G_s be the graph obtained from G' by removing the edges v_1a_i ($1 \leq i \leq d(v_1|G') - 2$) and adding the edges v_3a_i ($1 \leq i \leq d(v_1|G') - 2$). Clearly, G_s is a bipartite graph of order n , size $2n - 3$ with $\delta(G_s) \geq 2$ and $G_s \neq H_{n-6}^{3,3}$ because $\deg_{G_s}(a_{k_1}) = \deg_{G_s}(u_2) = 2$ and $|N_{G'}(a_{k_1}) \cap N_{G'}(u_2)| = 1$. Since $d(v_1|G') \leq k_1 + 1$, we have $|N_{G'}(v_3) \cap V_{3^+}^{G'}| \leq 1$. First let $|N_{G'}(v_3) \cap V_{3^+}^{G'}| = 0$. Then $d(v_1|G_s) = 2$ and $ABC(a_iv_1|G') = ABC(a_iv_3|G_s)$ for $1 \leq i \leq d(v_1|G') - 2$, and this implies that $ABC(G_s) \geq ABC(G') \geq ABC(G)$. It follows that $G_s \in G_n$ which contradicts Claim.

Now let $|N_{G'}(v_3) \cap V_{3^+}^{G'}| = 1$ and let $c \in N_{G'}(v_3) \cap V_{3^+}^{G'}$. Clearly, $ABC(a_iv_1|G') = ABC(a_iv_3|G_s)$ for any $1 \leq i \leq d(v_1|G') - 2$, $d(v_1|G_s) = 2$ and $d(c|G') = d(c|G_s)$. We write $d(c) = d(c|G')$. Let

$$\begin{aligned}
h_1 &= f(2, d(c)) - f(d(v_1|G'), d(c)) \\
&= \sum_{i=2^{d(v_1|G')-1}} (f(i, d(c)) - f(i+1, d(c)))
\end{aligned}$$

and

$$\begin{aligned}
h_2 &= f(d(v_3|G'), d(c)) - f(d(v_3|G') + d(v_1|G') - 2, d(c)) \\
&= \sum_{i=d(v_3|G')^{d(v_3|G') + d(v_1|G') - 3}} (f(i, d(c)) - f(i+1, d(c))).
\end{aligned}$$

Thus,

$$ABC(G_s) - ABC(G') \geq ABC(cv_1|G_s) + ABC(cv_3|G_s)$$

$$\begin{aligned}
& -ABC(cv_1|G') - ABC(cv_3|G') \\
& = f(d(v_1|G_s), d(c)) + f(d(v_3|G_s), d(c)) \\
& - f(d(v_1|G'), d(c)) - f(d(v_3|G'), d(c)) \\
& = f(2, d(c)) - f(d(v_1|G'), d(c)) \\
& - (f(d(v_3|G'), d(c)) - f(d(v_3|G'), d(c))) \\
& + d(v_1|G') - 2, d(c))) \\
& = h_1 - h_2 \\
& = \sum_{i=2^{d(v_1|G')-1}} (h(i, d(c)) \\
& - h(i + d(v_3|G') - 2, d(c))).
\end{aligned}$$

By Lemma 1, we have $h_1 - h_2 > 0$ and so $ABC(G_s) - ABC(G') > 0$. Hence $ABC(G_s) > ABC(G')$, which is a contradiction.

Subcase A.3. $k_2 = 0$ and $d(v_1|G') \geq k_1 + 2$.

Let G_s be the graph obtained from G' by removing the edges v_1a_i ($1 \leq i \leq k_1$) and adding the edges v_3a_i ($1 \leq i \leq k_1$). Clearly, G_s is a bipartite graph of order n , size $2n - 3$ with $\delta(G_s) \geq 2$.

First let $N_{G'}(v_3) \cap V_{3+}^{G'} = \emptyset$. Then $d(v_1|G_s) < d(v_1|G')$, $ABC(a_i v_1|G') = ABC(a_i v_3|G_s)$ for each $1 \leq i \leq k_1$, and $ABC(e|G_s) = ABC(e|G') = \frac{\sqrt{2}}{2}$ for any $e \in E_{v_3}^{G'}$. This implies that $ABC(G_s) \geq ABC(G')$. Because $L(G_s) = L(G') - |\{v_1, v_2\}| = L(G') - 1$, we obtain a contradiction with the choice of G' .

Now let $N_{G'}(v_3) \cap V_{3+}^{G'} \neq \emptyset$ and let $N_{G'}(v_3) \cap V_{3+}^{G'} = \{c_1, c_2, \dots, c_t\}$. Since $d(c_i|G') = d(c_i|G_s)$ for $i \in \{1, 2, \dots, t\}$, we write $d(c_i) = d(c_i|G')$. For $i \in \{1, 2, \dots, t\}$, let

$$\begin{aligned}
h_1^i & = f(d(v_1|G') - k_1, d(c_i)) - f(d(v_1|G'), d(c_i)) \\
& = \sum_{j=d(v_1|G')-k_1}^{d(v_1|G')-1} (f(j, d(c_i)) - f(j+1, d(c_i))) \\
& = \sum_{j=d(v_1|G')-k_1}^{d(v_1|G')-1} h(j, d(c_i)),
\end{aligned}$$

and

$$\begin{aligned}
h_2^i & = f(d(v_3|G'), d(c_i)) - f(d(v_3|G') + k_1, d(c_i)) \\
& = \sum_{j=d(v_3|G')^{d(v_3|G')+k_1-1}} (f(j, d(c_i)) - f(j+1, d(c_i))) \\
& = \sum_{j=d(v_3|G')^{d(v_3|G')+k_1-1}} h(j, d(c_i)).
\end{aligned}$$

Assume that $l = ABC(G_s) - ABC(G')$. We have

$$\begin{aligned}
l & \geq \sum_{i=1}^t (ABC(v_1c_i|G_s) + ABC(v_3c_i|G_s)) \\
& - \sum_{i=1}^t (ABC(v_1c_i|G') + ABC(v_3c_i|G'))
\end{aligned}$$

$$\begin{aligned}
& = \sum_{i=1}^t (ABC(v_1c_i|G_s) - ABC(v_1c_i|G')) \\
& - \sum_{i=1}^t (ABC(v_3c_i|G') - ABC(v_3c_i|G_s)) \\
& = \sum_{i=1}^t (f(d(v_1|G') - k_1, d(c_i)) - f(d(v_1|G'), d(c_i))) \\
& - \sum_{i=1}^t (f(d(v_3|G'), d(c_i)) - f(d(v_3|G') + k_1, d(c_i))) \\
& = \sum_{i=1}^t h_1^i - \sum_{i=1}^t h_2^i \\
& = \sum_{i=1}^t (h_1^i - h_2^i) \\
& = \sum_{i=1}^t \sum_{j=d(v_1|G')-k_1}^{d(v_1|G')-1} (h(j, d(c_i)) - h(j + d(v_3|G') \\
& - d(v_1|G') + k_1, d(c_i))).
\end{aligned}$$

We conclude from Lemma 1 and the fact $d(v_3|G') - d(v_1|G') + k_1 \geq 1$ that $l = ABC(G_s) - ABC(G') > 0$, which leads to a contradiction as above.

Subcase A.4. $0 < k_2 < k_1$.

Let G_s be the graph obtained from G' by removing the edges v_1a_i, v_3b_i ($1 \leq i \leq k_2$) and adding the edges v_1b_i, v_3a_i ($1 \leq i \leq k_2$). Clearly, G_s is a bipartite graph of order n , size $2n - 3$ with $\delta(G_s) \geq 2$. Note that $d(v|G_s) = d(v|G')$ for any $v \in G_s$ and $ABC(b_i v_1|G_s) \geq ABC(b_i v_3|G')$ for any $i = 1, 2, \dots, k_2$. It is not hard to verify that $ABC(G_s) \geq ABC(G')$ and $L(G_s) \leq L(G')$. Considering G_s instead of G' and applying the argument similar to that described in Subcases A.2 and A.3, we obtain a contradiction.

Case B. $|N_{G'}(u_1) \cap N_{G'}(u_2)| = 0$.

Let $N_{G'}(u_2) = \{v_3, v_4\}$ and assume without loss of generality that $d(v_2|G') \leq d(v_4|G')$. Define

$$\begin{aligned}
W_1 & = \{v \in V_2^{G'} | N_{G'}(v) = \{v_1, v_2\}\} = \{a_1 (= u_1), \dots, a_{q_1}\}, \\
W_2 & = \{v \in V_{3+}^{G'} | v_4 \in N_{G'}(v) \text{ and } v_2 \notin N_{G'}(v)\} \\
& = \{b_1, b_2, \dots, b_{q_2}\},
\end{aligned}$$

$$q_1 = |W_1| \text{ and } q_2 = |W_2|.$$

Obviously, $q_1 \geq 1$ and $q_2 \geq 0$. Now, we consider the following subcases.

Subcase B.1. $q_2 \geq q_1$.

Let G_s be the graph obtained from G' by removing the edges v_2a_i, v_4b_i ($1 \leq i \leq q_1$) and adding the edges v_4a_i, v_2b_i ($1 \leq i \leq q_1$). Clearly, G_s is a bipartite graph of order n , size $2n - 3$ with $\delta(G_s) \geq 2$ and $ABC(a_i v_2|G') = ABC(a_i v_4|G_s)$ for each $i \in \{1, 2, \dots, q_1\}$. Since $d(v_2|G') \leq d(v_4|G')$, we have $d(v_2|G_s) \leq d(v_4|G_s)$ and this implies that $ABC(b_i v_4|G') \leq ABC(b_i v_2|G_s)$ for any $i \in \{1, 2, \dots, q_1\}$.

Thus $ABC(G_s) \geq ABC(G')$. Clearly, $L(G_s) \leq L(G')$ and we deduce from the choice of G' that $L(G_s) = L(G')$. By definition, we have $G_s \neq H_{n-6}^{3,3}$. Thus $G_s \in H$ and we obtain a contradiction as in Case A.

Subcase B.2. $q_2 = 0$ and $d(v_2|G') \leq q_1 + 1$.

In this case, we have $d(v_2|G') - 2 \leq q_1 - 1$ and $|N(v_4|G') \cap V_{3+}^{G'}| \leq 1$. Let G_s be the graph obtained from G' by removing the edges $v_2a_i (1 \leq i \leq d(v_2|G') - 2)$ and adding the edges $v_4a_i (1 \leq i \leq d(v_2|G') - 2)$. Clearly, G_s is a bipartite graph of order n , size $2n - 3$ with $\delta(G_s) \geq 2$ and $G_s \neq H_{n-6}^{3,3}$. First let $|N_{G'}(v_4) \cap V_{3+}^{G'}| = 0$. We have $ABC(a_iv_2|G') = ABC(a_iv_4|G_s)$ for each $1 \leq i \leq d(v_2|G') - 2$, $d(v_2|G_s) = 2$ and $ABC(e|G_s) = ABC(e|G') = \frac{\sqrt{2}}{2}$ for any $e \in E_{v_4}^{G'}$. Hence $ABC(G_s) \geq ABC(G') \geq ABC(G)$ yielding $G_s \in G_n$, contradicting Claim 1, since $a_{q_1}v_2 \in E_{2,2}^{G_s}$.

Now let $|N_{G'}(v_4) \cap V_{3+}^{G'}| = 1$ and let $N_{G'}(v_4) \cap V_{3+}^{G'} = \{c\}$. Clearly, we have $ABC(a_iv_2|G') = ABC(a_iv_4|G_s)$ for each $1 \leq i \leq d(v_2|G') - 2$ and $d(v_2|G_s) = 2$. Since $d(c|G') = d(c|G_s)$, we write $d(c) = d(c|G')$. Assume that

$$\begin{aligned} h_1 &= f(2, d(c)) - f(d(v_2|G'), d(c)) \\ &= \sum_{i=2}^{d(v_2|G')-1} (f(i, d(c)) - f(i+1, d(c))), \\ h_2 &= f(d(v_4|G'), d(c)) - f(d(v_4|G') + d(v_2|G') - 2, d(c)) \\ &= \sum_{i=d(v_4|G') + d(v_2|G') - 3}^{d(v_4|G') + d(v_2|G') - 2} (f(i, d(c)) - f(i+1, d(c))). \end{aligned}$$

and $l = ABC(G_s) - ABC(G')$. Then we have

$$\begin{aligned} l &\geq ABC(cv_2|G_s) + ABC(cv_4|G_s) - (ABC(cv_2|G') \\ &\quad + ABC(cv_4|G')) \\ &= f(d(v_2|G_s), d(c)) + f(d(v_4|G_s), d(c)) - (f(d(v_2|G'), d(c)) \\ &\quad + f(d(v_4|G'), d(c))) \\ &= f(2, d(c)) - f(d(v_2|G'), d(c)) - (f(d(v_4|G'), d(c)) \\ &\quad - f(d(v_4|G') + d(v_2|G') - 2, d(c))) \\ &= h_1 - h_2 \\ &= \sum_{i=2}^{d(v_2|G')-1} (h(i, d(c)) - h(i + d(v_4|G') - 2, d(c))). \end{aligned}$$

We deduce from Lemma 1 that $ABC(G_s) - ABC(G') > 0$. This implies that $ABC(G_s) > ABC(G')$, which is a contradiction.

Subcase B.3. $q_2 = 0$ and $d(v_2|G') \geq q_1 + 2$.

Let G_s be the graph obtained from G' by removing the edges $v_2a_i (1 \leq i \leq q_1)$ and adding the edges $v_4a_i (1 \leq i \leq q_1)$. Clearly, G_s is a bipartite graph of order n , size $2n - 3$ with $\delta(G_s) \geq 2$ and $G_s \neq H_{n-6}^{3,3}$. First let $N_{G'}(v_4) \cap V_{3+}^{G'} = \emptyset$. Then we have $ABC(a_iv_2|G') =$

$ABC(a_iv_4|G_s)$ for any $1 \leq i \leq q_1$, $d(v_2|G_s) < d(v_2|G')$, and $ABC(e|G_s) = ABC(e|G') = \frac{\sqrt{2}}{2}$ for any edge $e \in E_{v_4}^{G'}$. Hence $ABC(G_s) \geq ABC(G')$ and $L(G_s) \leq L(G')$. We deduce from the choice of G' that $L(G_s) = L(G')$. Now, we consider G_s instead of G' and proceed as Case A to obtain a contradiction.

Now let $N_{G'}(v_4) \cap V_{3+}^{G'} \neq \emptyset$ and let $N_{G'}(v_4) \cap V_{3+}^{G'} = \{c_1, c_2, \dots, c_t\}$. Since $d(c_i|G') = d(c_i|G_s)$ for each $i \in \{1, 2, \dots, t\}$, we write $d(c_i) = d(c_i|G')$. Let

$$\begin{aligned} h_1^i &= f(d(v_2|G') - k_1, d(c_i)) - f(d(v_2|G'), d(c_i)) \\ &= \sum_{j=d(v_2|G')-k_1}^{d(v_2|G')-1} (f(j, d(c_i)) - f(j+1, d(c_i))) \\ &= \sum_{j=d(v_2|G')-k_1}^{d(v_2|G')-1} h(j, d(c_i)), \\ h_2^i &= f(d(v_4|G'), d(c_i)) - f(d(v_4|G') + k_1, d(c_i)) \\ &= \sum_{j=d(v_4|G') + k_1}^{d(v_4|G') + k_1 - 1} (f(j, d(c_i)) - f(j+1, d(c_i))) \\ &= \sum_{j=d(v_4|G') + k_1}^{d(v_4|G') + k_1 - 1} h(j, d(c_i)). \end{aligned}$$

and $l = ABC(G_s) - ABC(G')$. Then we have

$$\begin{aligned} l &\geq \sum_{i=1}^t (ABC(v_2c_i|G_s) + ABC(v_4c_i|G_s)) \\ &\quad - \sum_{i=1}^t (ABC(v_2c_i|G') + ABC(v_4c_i|G')) \\ &= \sum_{i=1}^t (ABC(v_2c_i|G_s) - ABC(v_2c_i|G')) \\ &\quad - \sum_{i=1}^t (ABC(v_4c_i|G') - ABC(v_4c_i|G_s)) \\ &= \sum_{i=1}^t (f(d(v_2|G') - k_1, d(c_i)) - f(d(v_2|G'), d(c_i))) \\ &\quad - \sum_{i=1}^t (f(d(v_4|G'), d(c_i)) - f(d(v_4|G') + k_1, d(c_i))) \\ &= \sum_{i=1}^t h_1^i - \sum_{i=1}^t h_2^i \\ &= \sum_{i=1}^t (h_1^i - h_2^i) \\ &= \sum_{i=1}^t \sum_{j=d(v_2|G')-k_1}^{d(v_2|G')-1} (h(j, d(c_i)) - h(j + d(v_4|G') \\ &\quad - d(v_2|G') + k_1, d(c_i))). \end{aligned}$$

It follows from Lemma 1 and the fact $d(v_4|G') - d(v_2|G') + k_1 \geq 1$ that $ABC(G_s) - ABC(G') > 0$. Thus $ABC(G_s) > ABC(G')$, which is a contradiction.

Subcase B.4. $0 < q_2 < q_1$.

Let G_s be the graph obtained from G' by removing the edges $v_2a_i, v_4b_i (1 \leq i \leq q_2)$ and adding the edges

$v_2 b_i, v_4 a_i (1 \leq i \leq q_2)$. Clearly, G_s is a bipartite graph of order n , size $2n - 3$ with $\delta(G_s) \geq 2$ and $G_s \neq H_{n-6}^{3,3}$. It is easy to verify that $ABC(G_s) \geq ABC(G')$ and $L(G_s) \leq L(G')$. Considering G_s instead of G' and applying the argument similar to that described in Subcases A.2 and A.3, we obtain a contradiction. This completes the proof of Claim 3. $\square$

Let $G' \neq H_{n-6}^{3,3}$ be the graph satisfying the conditions of Claim 3. Then $G' \in G_n$. By exchanging G and G' , we may assume that the graph G satisfies the conditions of Claim 3. Let

$$A_X = \{\{u, v\} \mid \text{there is a vertex } w \in Y \text{ such that } N(w) = \{u, v\}\},$$

$$A_Y = \{\{u, v\} \mid \text{there is a vertex } w \in X \text{ such that } N(w) = \{u, v\}\}.$$

By Claim 3, $|A_X| \leq 1$ and $|A_Y| \leq 1$. If $A_X \neq \emptyset$ (resp. $A_Y \neq \emptyset$), then let $A_X = \{\{u_x, v_x\}\}$ (resp. $A_Y = \{\{u_y, v_y\}\}$).

Claim 4. (a) If $A_X \neq \emptyset$, $|E_{u_x} \cap E_{3^+, 3^+}| + |E_{v_x} \cap E_{3^+, 3^+}| \leq 5$.
(b) If $A_Y \neq \emptyset$, $|E_{u_y} \cap E_{3^+, 3^+}| + |E_{v_y} \cap E_{3^+, 3^+}| \leq 5$.

Proof of Claim 4. We only prove (a). Let $A_X \neq \emptyset$. Suppose, to the contrary, that $|E_{u_x} \cap E_{3^+, 3^+}| + |E_{v_x} \cap E_{3^+, 3^+}| \geq 6$. Since G is a bipartite graph of size $2n - 3$, we conclude that $d(v) \leq n - 3$ for any $v \in V(G)$. Assume, without loss of generality, that $|E_{u_x} \cap E_{3^+, 3^+}| \geq 1$. Then there are two vertices $t, s \in Y$ such that $tu_x \in E_{3^+, 3^+}$ and $s \in N(u_x) \cap N(v_x) \cap V_2$. Let $E_1 = E_{u_x} \cap E_{3^+, 3^+}$ and $E_2 = E_{v_x} \cap E_{3^+, 3^+}$. Suppose $G' = G - s$. Clearly, G' is a bipartite graph of order $n - 1$, size $2(n - 1) - 3$ with $\delta(G') \geq 2$. By the choice of n , we have $ABC(G') \leq \sqrt{2}(n - 7) + 2\sqrt{\frac{3(n-3)}{n-4}} + 2$. Also, we have

$$\begin{aligned} ABC(tu_x|G') - ABC(tu_x|G) &= f(d(u_x) - 1, d(t)) \\ &\quad - f(d(u_x), d(t)) \\ &= h(d(u_x) - 1, d(t)) \\ &\geq h(n - 4, d(t)) \\ &\geq h(n - 4, 3). \end{aligned}$$

Similarly, for any edge $e \in E_1 \cup E_2$, we have $ABC(e|G') - ABC(e|G) \geq h(n - 4, 3)$. Hence

$$\begin{aligned} ABC(G') + \sqrt{2} - ABC(G) &= \sum_{e \in E_1 \cup E_2} (ABC(e|G') - ABC(e|G)) \\ &\geq (|E_1| + |E_2|)h(n - 4, 3) \\ &\geq 6h(n - 4, 3) \\ &= ABC(H_{n-7}^{3,3}) + \sqrt{2} - ABC(H_{n-6}^{3,3}). \end{aligned}$$

Since $ABC(G) \geq ABC(H_{n-6}^{3,3})$, we have

$$ABC(H_{n-7}^{3,3}) + \sqrt{2} - ABC(H_{n-6}^{3,3}) \geq ABC(G') + \sqrt{2} - ABC(G)$$

$$\begin{aligned} &\geq ABC(H_{n-7}^{3,3}) + \sqrt{2} \\ &\quad - ABC(H_{n-6}^{3,3}) \end{aligned}$$

and so the inequalities occurring above become equality, that is, $ABC(G) = ABC(H_{n-6}^{3,3})$ and $ABC(G') = ABC(H_{n-7}^{3,3})$. It follows that $G' \cong H_{n-7}^{3,3}$ and $ABC(e|G') - ABC(e|G) = h(n - 4, 3)$ for any $e \in E_1 \cup E_2$. Hence $d(u_x) = d(v_x) = n - 3$ and so $G \cong H_{n-6}^{3,3}$, a contradiction. $\square$

Claim 5. $k \leq 9$.

Proof of Claim 5. Suppose, to the contrary, that $k \geq 10$. Let $q = |A_X| + |A_Y|$. By Claim 4, we have $q \in \{0, 1, 2\}$. Let $B = \{u_x, v_x, u_y, v_y\}$ (possibly $B = \emptyset$). Then $|B| = 2q$. We consider the following cases.

Case C.I. There exists a vertex $v \notin B$ such that $d(v) \geq 6$. Then

$$\begin{aligned} ABC(G) &= \sum_{e \in E_{2,3^+}} ABC(e) + \sum_{e \in E_v} ABC(e) \\ &\quad + \sum_{e \in \{E_{3^+, 3^+} \setminus E_v\}} ABC(e) \\ &\leq (n - k)\sqrt{2} + d(v)\sqrt{\frac{d(v) + 1}{3d(v)}} + (2k - 3 - d(v))\frac{2}{3} \\ &= (n - k)\sqrt{2} + (2k - 3)\frac{2}{3} - d(v)\left(\frac{2}{3} - \sqrt{\frac{d(v) + 1}{3d(v)}}\right) \\ &\leq (n - k)\sqrt{2} + (2k - 3)\frac{2}{3} - 6\left(\frac{2}{3} - \sqrt{\frac{7}{18}}\right) \\ &\leq (n - 10)\sqrt{2} + (20 - 3)\frac{2}{3} - 6\left(\frac{2}{3} - \sqrt{\frac{7}{18}}\right) \\ &\leq (n - 6)\sqrt{2} + 2 + 2\sqrt{3} \\ &< (n - 6)\sqrt{2} + 2 + 2\sqrt{\frac{3(n-2)}{n-3}} \\ &= ABC(H_{n-6}^{3,3}), \end{aligned}$$

a contradiction.

Case C.II. There exist two vertices $v_1, v_2 \notin B$ such that $d(v_1) = 5$ and $d(v_2) \geq 4$.

Let $t_1 = |E_{v_1} \cap E_{v_2}|$. Then $t_1 \in \{0, 1\}$ and

$$\begin{aligned} h_1 &= t_1\left(\sqrt{\frac{3 + d(v_2)}{5d(v_2)}} - \sqrt{\frac{6}{15}} - \sqrt{\frac{d(v_2) + 1}{3d(v_2)}} + \frac{2}{3}\right) \\ &= t_1(f(3, 3) - f(d(v_2), 3) - (f(3, 5) - f(d(v_2), 5))) \\ &= t_1\left(\sum_{j=1}^{d(v_2)-1} h(j, 3) - \sum_{j=1}^{d(v_2)-1} h(j, 5)\right) \\ &\leq 0. \end{aligned}$$

It follows that

$$\begin{aligned}
 ABC(G) &= \sum_{e \in E_{2,3^+}} ABC(e) + \sum_{e \in E_{v_1}} ABC(e) \\
 &+ \sum_{e \in E_{v_2} \setminus E_{v_1}} ABC(e) + \sum_{e \in \{E_{3^+,3^+} \setminus (E_{v_1} \cup E_{v_2})\}} ABC(e) \\
 &\leq (n-k)\sqrt{2} + t_1 \sqrt{\frac{3+d(v_2)}{5d(v_2)}} + (5-t_1) \sqrt{\frac{6}{15}} \\
 &+ (d(v_2) - t_1) \sqrt{\frac{d(v_2)+1}{3d(v_2)}} + (2k-8-d(v_2)+t_1) \frac{2}{3} \\
 &= h_1 + (n-k)\sqrt{2} + 5\sqrt{\frac{6}{15}} + d(v_2) \sqrt{\frac{d(v_2)+1}{3d(v_2)}} \\
 &+ (2k-8-d(v_2)) \frac{2}{3} \\
 &\leq (n-k)\sqrt{2} + 5\sqrt{\frac{6}{15}} - d(v_2) \left(\frac{2}{3} - \sqrt{\frac{d(v_2)+1}{3d(v_2)}} \right) \\
 &+ (2k-8) \frac{2}{3} \\
 &\leq (n-10)\sqrt{2} + 5\sqrt{\frac{6}{15}} - 4 \left(\frac{2}{3} - \sqrt{\frac{4+1}{12}} \right) \\
 &+ (2k-8) \frac{2}{3} \\
 &\leq (n-6)\sqrt{2} + 2 + 2\sqrt{3} \\
 &< (n-6)\sqrt{2} + 2 + 2\sqrt{\frac{3(n-2)}{n-3}} \\
 &= ABC(H_{n-6}^{3,3}),
 \end{aligned}$$

which is a contradiction.

Case C.III. There exist two vertices $u, v \notin B$ such that $d(v) = 5$ and $d(x) = 3$ for any $x \in V_{3^+} \setminus \{v\}$.

By Claim 4, we have

$$\begin{aligned}
 \sum_{v \in V_{3^+}} d(v|G[V_{3^+}]) &= \sum_{v \in V_{3^+} \setminus B} d(v|G[V_{3^+}]) + \sum_{v \in B} d(v|G[V_{3^+}]) \\
 &\leq 5 + 3(k-2q-1) + 5q \\
 &= 2 + 3k - q \\
 &\leq 2 + 3k.
 \end{aligned}$$

By Claim 1, we have $\sum_{v \in V_{3^+}} d(v|G[V_{3^+}]) = \sum_{v \in V_{3^+}} d(v) = 2(2k-3) \leq 2 + 3k$ yielding $k \leq 8$, which is a contradiction.

Case C.IV. There are three vertices $v_1, v_2, v_3 \notin B$ such that $d(v_1) = d(v_2) = d(v_3) = 4$.

Let W be the set of edges with two ends in $\{v_1, v_2, v_3\}$, $t_1 = |W|$ and $W_1 = (E_{v_1} \cup E_{v_2} \cup E_{v_3}) \setminus W$. Clearly, $t_1 \in \{0, 1, 2\}$ and we have

$$ABC(G) = \sum_{e \in E_{2,3^+}} ABC(e) + \sum_{e \in W} ABC(e) + \sum_{e \in W_1} ABC(e)$$

$$\begin{aligned}
 &+ \sum_{e \in \{E_{3^+,3^+} \setminus \{W \cup W_1\}\}} ABC(e) \\
 &\leq (n-k)\sqrt{2} + t_1 \sqrt{\frac{6}{16}} + (12-2t_1) \sqrt{\frac{5}{12}} \\
 &+ (2k-3-12+t_1) \frac{2}{3} \\
 &= t_1 \left(\sqrt{\frac{6}{16}} - 2\sqrt{\frac{5}{12}} + \frac{2}{3} \right) + (n-k)\sqrt{2} \\
 &+ 12\sqrt{\frac{5}{12}} + (2k-15) \frac{2}{3} \\
 &\leq (n-k)\sqrt{2} + 12\sqrt{\frac{5}{12}} + (2k-15) \frac{2}{3} \\
 &\leq (n-10)\sqrt{2} + 12\sqrt{\frac{5}{12}} + (20-15) \frac{2}{3} \\
 &\leq (n-6)\sqrt{2} + 2 + 2\sqrt{3} \\
 &< (n-6)\sqrt{2} + 2 + 2\sqrt{\frac{3(n-2)}{n-3}} \\
 &= ABC(H_{n-6}^{3,3}),
 \end{aligned}$$

a contradiction.

Case C.V. For any vertex $v \notin B$, $d(v) \leq 4$ and $|\{v|d(v) = 4\} \cap (V_{3^+} \setminus B)| \leq 2$.

By claim 4, we have

$$\begin{aligned}
 \sum_{v \in V_{3^+}} d(v|G[V_{3^+}]) &= \sum_{v \in V_{3^+} \setminus B} d(v|G[V_{3^+}]) + \sum_{v \in B} d(v|G[V_{3^+}]) \\
 &\leq 8 + 3(k-2q-2) + 5q \\
 &= 2 + 3k - q \\
 &\leq 2 + 3k.
 \end{aligned}$$

Claim 1 implies that $\sum_{v \in V_{3^+}} d(v|G[V_{3^+}]) = \sum_{v \in V_{3^+}} d(v) = 2(2k-3) \leq 2 + 3k$ yielding $k \leq 8$, a contradiction. This completes the proof of Claim 5. $\square$

Now, for any graph G'' , we define $d'(u) = \begin{cases} d(u) & d(u) \geq 3 \\ 4 & d(u) \leq 2 \end{cases}$,

$$ABC'(uv) = \sqrt{\frac{d'(u)+d'(v)-2}{d'(u)d'(v)}} \quad \text{and} \quad ABC'(G'') = \sum_{uv \in E(G'')} ABC'(uv).$$

By Claims 1 and 2, $|E_{2,2}^G| = |E_{2,3}^G| = 0$. We have $d(v) \geq 4$ with $d(v|G[V_{3^+}]) \leq 2$ for any $v \in V_{3^+}$. Thus $ABC(G) \leq (n-k)\sqrt{2} + ABC'(G[V_{3^+}])$.

Claim 6. $k = 6$.

Proof of Claim 6. Suppose, to the contrary, that $k \geq 7$. First let $k = 9$. Then $ABC(G) \leq (n-9)\sqrt{2} + ABC'(G[V_{3^+}])$. Since $ABC(G) \geq ABC(H_{n-6}^{3,3}) > (n-6)\sqrt{2} + 2\sqrt{3} + 2$, we obtain $ABC'(G[V_{3^+}]) > 3\sqrt{2} + 2\sqrt{3} + 2$. Hence, $|V(G[V_{3^+}])| = 9$, $|E(G[V_{3^+}])| = 15$ and $ABC'(G[V_{3^+}]) > 3\sqrt{2} + 2\sqrt{3} + 2$. A computer search shows that there are exactly two bipartite

graphs G'' satisfying the conditions $|V(G'')| = 9$, $|E(G'')| = 15$ and $ABC'(G'') > 3\sqrt{2} + 2\sqrt{3} + 2$ (these two graphs G_9^1 and G_9^2 illustrated in Figure 2). It is easy to verify that $d(u) + d(v) \geq 6$ for every two vertices $u, v \in V(G_9^1)$ or $u, v \in V(G_9^2)$, a contradiction with Claim 4.

Now let $k = 8$. Then $ABC(G) \leq (n-8)\sqrt{2} + ABC'(G[V_{3+}])$. Since $ABC(G) \geq ABC(H_{n-6}^{3,3}) > (n-6)\sqrt{2} + 2\sqrt{3} + 2$, we have $ABC'(G[V_{3+}]) > 2\sqrt{2} + 2\sqrt{3} + 2$. Thus $G[V_{3+}]$ satisfies the following $|V(G[V_{3+}])| = 8$, $|E(G[V_{3+}])| = 13$ and $ABC'(G[V_{3+}]) > 2\sqrt{2} + 2\sqrt{3} + 2$. A computer search shows that there are exactly two bipartite graphs G'' satisfying the conditions $|V(G'')| = 8$, $|E(G'')| = 13$ and $ABC'(G'') > 2\sqrt{2} + 2\sqrt{3} + 2$ (these two graphs G_8^1 and G_8^2 illustrated in Figure 2). If $G[V_{3+}] = G_8^1$, then it is easy to verify $d(u) + d(v) \geq 6$ for every two vertices $u, v \in V(G_8^1)$, a contradiction with Claim 4. If $G[V_{3+}] = G_8^2$, then let u be the vertex of degree 2, and assume without loss of generality that $u \in X$. Suppose $v \in X$ be a vertex of degree 3. By Claim 4, we conclude that G is a graph obtained from G_8^2 by adding vertices $a_1, a_2, \dots, a_{n-8}$ and the edges $a_i u, a_i v$ for each $i \in \{1, 2, \dots, n-8\}$ (See graph F_8 in Figure 3). It is not hard to verify that $ABC(G) < ABC(H_{n-6}^{3,3})$, a contradiction.

Finally let $k = 7$. A computer search shows that there are exactly two bipartite graphs G'' satisfying the conditions $|V(G'')| = 7$, $|E(G'')| = 11$. We deduce from Claim 4 that G is a graph obtained from G'' by adding new vertices $v_1, v_2, \dots, v_{n-7}$ and joining them to two vertices $u, v \in X_{G''}$ (see the graph F_7 illustrated in Figure 3). It is easy to verify that $ABC(F_7) < ABC(H_{n-6}^{3,3})$, a contradiction. This completes the proof of Claim 6.

Figure 2: Graphs used in the proof of Claim 6.

Figure 3: Graphs constructed in the proof of Claim 6.

Claim 7. For any graph G_s with $|V(G_s)| = n$, $|E(G_s)| = 2n - 3$, $|\delta(G_s)| \geq 2$, and $ABC(G_s) \geq ABC(G)$, we have $G_s[V_{3+}] \cong K_{3,3}$ and $|\bigcup_{u \in V_{2+}^{G_s} \cap Y_{G_s}} N_{G_s}(u)| \in \{0, 2\}$ and $|\bigcup_{u \in V_{2+}^{G_s} \cap X_{G_s}} N(u)| \in \{0, 2\}$.

Proof of Claim 7. Note that $E_{2,2}^{G_s} = E_{2,3}^{G_s} = \emptyset$. Then by Claim 6, we have $G_s[V_{3+}] \cong K_{3,3}$. By above Claims, we only need to show $|\bigcup_{u \in V_{2+}^{G_s} \cap Y_{G_s}} N_{G_s}(u)| \in \{0, 2\}$. Since $E_{2,2}^{G_s} = E_{2,3}^{G_s} = \emptyset$, we have $N_{G_s}(u) \cap V_{3+}^{G_s} \neq \emptyset$ for any $u \in V(G)$. Since $G_s[V_{3+}] \cong K_{3,3}$, we have $N_{G_s}(u) \cap V_{3+}^{G_s} = N_{G_s}(v) \cap V_{3+}^{G_s} \neq \emptyset$ for any $u, v \in X \cap V_{3+}^{G_s}$. Then, by a close look at the proof of Case A in Claim 3, we have $|\bigcup_{u \in V_{2+}^{G_s} \cap Y_{G_s}} N_{G_s}(u)| \in \{0, 2\}$. $\square$

Let $t = |\bigcup_{u \in V_2 \cap Y} N(u)| + |\bigcup_{u \in V_2 \cap X} N(u)|$. We conclude from Claim 7 and the fact $n \geq 10$ that $t \in \{2, 4\}$. If $t = 2$, then $G \cong ABC(H_{n-6}^{3,3})$, a contradiction. Let $t = 4$. Assume that $\{u_x, v_x\} = \bigcup_{u \in V_2 \cap Y} N(u)$, $\{u_y, v_y\} = \bigcup_{u \in V_2 \cap X} N(u)$, $U_1 = \{v | N(v) = \{u_x, v_x\}\}$, $U_2 = \{v | N(v) = \{u_y, v_y\}\}$, $\{u_1\} = X - (\{u_x, v_x\} \cup V_2)$, $\{u_2\} = Y - (\{u_y, v_y\} \cup V_2)$ and $d(u_y) \leq d(u_x)$. Let $t \in U_2$, and let G' be the bipartite graph obtained from $G - \{tu_y, tv_y\}$ by adding the edges tu_x and tv_x . Let $h_1 = 4ABC(u_x u_y | G') - 4ABC(u_x u_y | G)$ and

$$h_2 = 2ABC(u_1 u_y | G') - 2ABC(u_1 u_y | G) + 2ABC(u_2 u_x | G') - 2ABC(u_2 u_x | G).$$

Then $h_1 = 4 \left(\sqrt{\frac{d(u_x) + d(u_y) - 2}{(d(u_x) + 1)(d(u_y) - 1)}} - \sqrt{\frac{d(u_x) + d(u_y) - 2}{d(u_x)d(u_y)}} \right)$ and

$$\begin{aligned} h_2 &= 2ABC(u_1 u_y | G') - 2ABC(u_1 u_y | G) \\ &\quad + 2ABC(u_2 u_x | G') - 2ABC(u_2 u_x | G) \\ &= 2(f(d(u_y) - 1, 3) - f(d(u_y), 3) + f(d(u_x), 3) \\ &\quad - f(d(u_x) + 1, 3)) \\ &= 2(h(d(u_y) - 1, 3) - h(d(u_x), 3)). \end{aligned}$$

Since $d(u_y) \leq d(u_x)$, we have $h_1 > 0$ and $h_2 > 0$. Thus

$$\begin{aligned} ABC(G') - ABC(G) &= 4ABC(u_x u_y | G') - 4ABC(u_x u_y | G) \\ &\quad + 2ABC(u_1 u_y | G') - 2ABC(u_1 u_y | G) \\ &\quad + 2ABC(u_2 u_x | G') - 2ABC(u_2 u_x | G) \\ &= h_1 + h_2 \\ &> 0, \end{aligned}$$

a contradiction.

This completes the proof. $\square$

By applying the approach used above, we also obtain the following result:

Theorem 6. Let $-3 \leq l \leq -1$ and let G be a bipartite graph of order $n \geq l + 9$, size $2n + l$ and $\delta(G) \geq 2$. Then $ABC(G) \leq \sqrt{2}(n - 9 - l) + \sqrt{\frac{(l+6)(l+7)}{3}} + 2(l+6)\sqrt{\frac{n-2}{3(n-3)}}$, with equality if and only if $G \cong H_{n-l-9}^{3,l+6}$.

3 Discussions

We studied the atom–bond connectivity (ABC) index on bipartite graphs, in which the ABC index has an important application in rationalizing the stability of linear and branched alkanes as well as the strain energy of cycloalkanes. All extremal graphs attained at these extremal values are characterized. Our method is to use monotonic functions and combine them with graph operations. Some special graphs and their values are obtained by computational searches. Our results extend the previous outcomes and deduce all bounds.

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