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On the Maximum ABC Index of Graphs With Prescribed Size and Without Pendent Vertices

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ABSTRACT The atom-bond connectivity (ABC) index is one of the most actively studied degree-based graph invariants, which are found in a vast variety of chemical applications. For a simple graph G, it is defined as $ABC(G) = \sum_{uv\in E(G)}((d(u) + d(v) - 2)/(d(u)d(v)))^{1/2}$, where $d(v)$ denotes the degree of a vertex v of G. Recently in [17] graphs with n vertices, $2n - 4$ and $2n - 3$ edges, and maximum ABC index were characterized. Here, we consider the next, more complex case, and characterize the graphs with n vertices, $2n - 2$ edges, and maximum ABC index.

INDEX TERMS Atom–bond connectivity index, ABC index, extremal graph.

I. INTRODUCTION

Here only graphs without multiple edges or loops will be considered. For a graph G, the set of vertices of G is denoted by $V(G)$, and the set of edges of G by $E(G)$. For a subset S of $V(G)$, we denote by $G[S]$ the subgraph induced by S. A graph G is called an (n, m)-graph if G has n vertices and m edges. A complete graph of order n is denoted by K_n. The degree of a vertex v in G is denoted by $d_G(v)$ (or simply $d(G)$). An edge uv is an (s, t)-edge if $d(u) = s$ and $d(v) = t$. An edge uv is an (s^+, t^+)-edge if $d(u) \geq s$ and $d(v) \geq t$. A vertex u is said to be a neighbor of v if u is adjacent to v in G. We denote by $N(v)$ the set of neighbors of a vertex v. A vertex v is a *leaf* if $d(v) = 1$. Two distinct edges are adjacent if they have a common end-vertex. We denote by $L(v)$ and $\delta(G)$ the set of leaf neighbors of v and the minimum degree of G, respectively. We denote by $K_{s,t}$ the complete bipartite graph with two part sizes s and t.

For a graph G, a positive integer s, and $a, b \in V(G)$, we define a graph $T(G, a, b, s)$ by $V(T(G, a, b, s)) = V(G) \cup \{q_1, q_2, \ldots, q_s\}$, and $E(T(G, a, b, s)) = E(G) \cup \{q_1a, q_2a, \ldots, q_sa\} \cup \{q_1b, q_2b, \ldots, q_sb\}$. That is to say, $T(G, a, b, s)$ is obtained from G by adding s vertices of degree two adjacent to both a and b. For an example, see Figure 5 in [17].

The atom-bond connectivity (ABC) index of a graph G is defined as

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

Estrada *et al.* [10] proposed this vertex-degree-based graph topological index. They showed that the ABC index can be a valuable predictive tool in the study of the heat formation in alkanes. Ten years later, Estrada elaborated in [11] an innovative quantum-theory-like explanation of this topological index. Incontestably, this topic has triggered tremendous interest in both mathematical and chemical research communities, leading to a number of results that incorporate the structural properties and the computational aspects of the graphs with extremal properties [1], [3]–[9], [12], [16], [18], [19], [21]. On the other hand, the physico-chemical applicability of the ABC index has also been confirmed and extended in several other studies [2], [13]–[15], [20].

It has been proven that deleting/adding an edge in a graph strictly decreases/increases its ABC index [1], [4]. Consequently, among all connected graphs, a tree/the complete graph has minimal/maximal ABC index.

It has been shown that among the trees of a given order, the star is the one with a maximal ABC index [12].

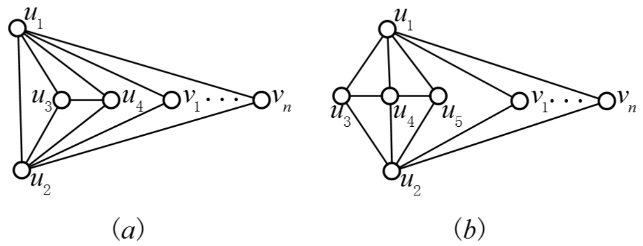

FIGURE 1. (a) The graph X_1^n; (b) the graph X_2^n.

Notwithstanding, a thoroughgoing characterization of trees with minimal ABC index, also referred to as minimal-ABC trees, still remains an open problem.

Another very difficult extremal problem is to determine which graphs with no pendent vertices have a maximal ABC index. In [17] two special instances of the above problem were considered: characterizing the maximal-ABC graphs with $2n-4$ and $2n-3$ edges, where n is the number of the vertices. The first problem is significantly easier, and by the second one it can be seen how the complexity of the problem increases even by adding only one edge more as in the first case. Here, we go a step further, as we take into consideration the case when the graph has $2n-2$ edges, the case, which is more difficult to analyze than the above two cases.

II. MAIN RESULTS

We then define graph X_1^n with $n+4$ vertices and $2n+6$ edges ($n \geq 1$) as follows: $V(X_1^n) = \{u_1, u_2, u_3, u_4, v_1, v_2, \cdots, v_n\}$ and $E(X_1^n) = \{u_1v_i, u_2v_i : 1 \leq i \leq n\} \cup \{u_1u_2, u_1u_3, u_1u_4, u_2u_3, u_2u_4, u_3u_4\}$. Similarly, we define graph X_2^n with $n+5$ vertices and $2n+8$ edges ($n \geq 2$) as follows: $V(X_2^n) = \{u_1, u_2, u_3, u_4, u_5, v_1, v_2, \cdots, v_n\}$ and $E(X_2^n) = \{u_1v_i, u_2v_i : 1 \leq i \leq n\} \cup \{u_1u_3, u_1u_4, u_1u_5, u_2u_3, u_2u_4, u_2u_5, u_3u_4, u_4u_5\}$. The graphs X_1^n and X_2^n are shown in Figure 1.

The following lemma is easy to verify:

Lemma 1: If $n \geq 5$, we have

i) $ABC(X_1^{n-4}) = \frac{\sqrt{2n-4}}{n-1} + 4\sqrt{\frac{n}{3(n-1)}} + (n-4)\sqrt{2} + \frac{2}{3}$;

ii) $ABC(X_2^{n-5}) = 4\sqrt{\frac{n-1}{3(n-2)}} + 2\sqrt{\frac{n}{4(n-2)}} + (n-5)\sqrt{2} + 2\sqrt{\frac{5}{12}}$;

iii) If $n \leq 34$, then $ABC(X_1^{n-4}) > ABC(X_2^{n-5})$, else $ABC(X_1^{n-4}) < ABC(X_2^{n-5})$.

Now we will define a family of graphs $\mathcal{G}$ as follows. For any graph G, $G \in \mathcal{G}$ if and only if G satisfies the conditions:

C1) G is a graph with minimum degree at least two on $n \geq 10$ vertices and $m = 2n-2$ edges.

C2) $G \ncong X_1^{n-4}$ and $G \ncong X_2^{n-5}$.

C3) G is a graph with the maximum ABC index, i.e.,

$$ABC(G) = \max\{ABC(H) | \delta(H) \geq 2, |V(H)| = n\}.$$

C4) G satisfies the conditions C1, C2 and C3 with the minimum number of vertices, i.e., $|V(G)|$ is as small as possible.

For a graph $G = (V, E)$, we use the following notations to prove the theorems.

$N'(e)$: the set of edges adjacent to the edge e,

E_v : the set of edges incident to the vertex v,

$V_i = \{v | d(v) = i\}$ for $i \geq 2$,

$V_{3^+} = \{v | d(v) \geq 3\}$, $k = |V_{3^+}|$ and $V_{3^+} = \{u_1, u_2, \cdots, u_k\}$,

$n_2 = |V_2|$,

$V'_3 = \{v | d_{G[V_{3^+}]}(v) = 3\}$,

$E_{s,t} = \{uv | d(u) = s, d(v) = t\}$,

$E_{s,t^+} = \{uv | d(u) = s, d(v) \geq t\}$,

$E_{s^+,t^+} = \{uv | d(u) \geq s, d(v) \geq t\}$,

$\ell_1 = |E_{2,2}|$, $\ell_2 = |E_{2,3^+}|$, $\ell_3 = |E_{3^+,3^+}|$,

$E'_{3,3} = \{uv | d_{G[V_{3^+}]}(u) = 3, d_{G[V_{3^+}]}(v) = 3\}$.

That is to say, V'_3 is the set of vertices with degree three in $G[V_{3^+}]$ and $E'_{3,3}$ the set of edges whose end vertices have degree three in $G[V_{3^+}]$.

Lemma 2: For any (n, m)-graph G with $n \geq 10$ and $m = 2n-2$ and $\delta(G) \geq 2$, we have

a) $\ell_3 = 2k - 2 + \ell_1$;

b) $\ell_3 \geq 6$ and $k \geq 4$.

Proof: a) Via the summation of the degrees of all the vertices, we have

$$\sum_{v \in V_2} d(v) + \sum_{v \in V_{3^+}} d(v) = 2n_2 + \sum_{i=1}^{k} d(u_i) = 2m = 4n-4, 5 \tag{1}$$

$$n = n_2 + k, \tag{2}$$

and

$$2n-2 = \ell_1 + \ell_2 + \ell_3. \tag{3}$$

By Eq. (1)-(3), we have

$$-2k + \sum_{i=1}^{k} d(u_i) = 2n-4. \tag{4}$$

Since $\sum_{i=1}^{k} d(u_i) = \ell_2 + 2\ell_3$, we have

$$\ell_3 = 2k - 2 + \ell_1. \tag{5}$$

b) If $k = 0$, then G is the union of cycles, contradicting with $m = 2n-2$. Hence we have $k \geq 1$.

Now, we claim that $\ell_3 \geq 3$. Otherwise, suppose on the contrary that $\ell_3 \leq 2$, then we have $\ell_3 = 2k - 2 + \ell_1 \leq 2$. Hence we have $\ell_1 \leq 4 - 2k \leq 2$.

Case 1 ($\ell_3 = 0$): In this case, we have $k = 1$ and $\ell_1 = 0$. This means that there is exactly one vertex with degree at least three and the other vertices with degree two. It is clear that such a graph does not exist.

Case 2 ($\ell_3 = 1$): In this case, we have $k = 1$. This means that there is exactly one vertex with degree at least three. Therefore, there is no edge $e \in E_{3^+,3^+}$, a contradiction.

Case 3 ($\ell_3 = 2$): In this case, we have $k \leq 2$. This means that there are at most two vertices with degree at least three. Therefore, there is at most one edge $e \in E_{3^+,3^+}$, which is a contradiction.

From above, we have $\ell_3 \geq 3$. Hence, $k \geq 3$. Now we will show that $k \neq 3$. Otherwise, there are at most three edges $e_1, e_2, e_3 \in E_{3^+,3^+}$, i.e., $\ell_3 \leq 3$. By Eq. (5), we have $\ell_3 = 2k-2+\ell_1 \geq 2k-2 \geq 4$, a contradiction.

Now from above, we have $k \geq 4$, and thus $\ell_3 = 2k-2+\ell_1 \geq 2k-2 \geq 6$. This assertion completes the proof. □

Lemma 3: If G is an (n, m)-graph with $n \geq 10, m = 2n-2$, $\delta(G) \geq 2$ and G has the maximum ABC index, then $|E_{2,2}| = 0$.

Proof: We first prove the following claim:

Claim 1: there is an edge $e \in E_{3^+,3^+}$ such that $e \notin E_v$ for any $v \in V_{3^+}$.

Proof: Otherwise, $\ell_3 \leq k-1$. By Eq. (5), we have $\ell_3 = 2k-2+\ell_1$. So we have $2k-2+\ell_1 \leq k-1$ and thus $k-1+\ell_1 \leq 0$. By Lemma 2, we have $k \geq 4$, a contradiction with $k-1+\ell_1 \leq 0$. □

Now, suppose on the contrary that $|E_{2,2}| \geq 1$, this way there is an edge $w_1v_1 \in E_{2,2}$. By Lemma 2, we have $\ell_3 \geq 6$, and thus, there is an edge $w_2v_2 \in E_{3^+,3^+}$ such that w_1v_1 and w_2v_2 are disjoint. Since $d(w_1) = 2$, without loss of generality we may assume that $w_1w_2 \notin E(G)$. We consider the following cases.

Case 1 ($v_1v_2 \notin E(G)$): We now consider a graph G' such that $G' = G - w_1v_1 - w_2v_2 + w_1w_2 + v_1v_2$. It can be seen that $ABC(G') > ABC(G)$, a contradiction.

Case 2 ($v_1v_2 \in E(G)$ and $w_1v_2 \notin E(G)$): Since $d(v_1) = 2$, we have $v_1w_2 \notin E(G)$. We now consider a graph G' such that $G' = G - w_1v_1 - w_2v_2 + w_1v_2 + w_2v_1$. It can be seen that $ABC(G') > ABC(G)$, a contradiction.

Case 3 ($v_1v_2 \in E(G)$ and $w_1v_2 \in E(G)$): By Claim 1, we have that there is an edge $w_3v_3 \in E_{3+3+}$ such that v_2 is not incident to w_3v_3. Since $w_1v_1 \in E_{2,2}$, we can conclude that w_1v_1 and w_3v_3 are disjoint. Now, applying the proof of Case 1 for w_3v_3 and w_2v_2 we obtain a contradiction. □

Lemma 4: If $G \in \mathcal{G}$, then $|E_{2,3}| = 0$.

Proof: Suppose on the contrary that there is an edge $w_1v_1 \in E_{2,3}$, we have w_1 has another neighbor $v_3 \in V_{3^+}$ by Lemma 3.

Case 1: there is a vertex $v_2 \in N(v_1)$ with $v_2 \in V_{3^+}$.

Let $G' = G - \{w_1\}$, then we have $ABC(e|G) \leq ABC(e|G')$ for any $e \in E(G')$, and $x = d(v_2)$. Then we have

$$ABC(w_1v_1|G) = ABC(w_1v_3|G) = ABC(v_1v_2|G') = \frac{\sqrt{2}}{2},$$

and

$$ABC(v_1v_2|G) = \sqrt{\frac{x+1}{3x}}.$$

Therefore, we have

$$\begin{aligned} ABC(G) &\leq ABC(G') + ABC(w_1v_1|G) \\ &\quad + ABC(w_1v_3|G) + ABC(v_1v_2|G) \\ &\quad - ABC(v_1v_2|G') \\ &\leq ABC(G') + \sqrt{2} - \left(\frac{\sqrt{2}}{2} - \sqrt{\frac{x+1}{3x}}\right) \\ &\leq ABC(G') + \sqrt{2} - \left(\frac{\sqrt{2}}{2} - \frac{2}{3}\right). \end{aligned}$$

Subcase 1.1 ($ABC(G') \leq ABC(X_1^{n-5})$): In this case, we have if $n \geq 10$, then

$$\begin{aligned} ABC(G) &\leq ABC(X_1^{n-5}) + \sqrt{2} - \left(\frac{\sqrt{2}}{2} - \frac{2}{3}\right) \\ &= ABC(X_1^{n-4}) \\ &\quad -4\left(\sqrt{\frac{n}{3(n-1)}} - \sqrt{\frac{n-1}{3(n-2)}}\right) \\ &\quad -\left(\frac{\sqrt{2n-4}}{n-1} - \frac{\sqrt{2n-6}}{n-2}\right) - \left(\frac{\sqrt{2}}{2} - \frac{2}{3}\right) \\ &< ABC(X_1^{n-4}), \end{aligned}$$

a contradiction.

Subcase 1.2 ($ABC(G') \leq ABC(X_2^{n-6})$): In this case, we have if $n \geq 10$, then

$$\begin{aligned} ABC(G) &\leq ABC(X_2^{n-6}) + \sqrt{2} - \left(\frac{\sqrt{2}}{2} - \frac{2}{3}\right) \\ &= ABC(X_2^{n-5}) \\ &\quad -4\left(\sqrt{\frac{n-1}{3(n-2)}} - \sqrt{\frac{n-2}{3(n-3)}}\right) \\ &\quad -2\left(\sqrt{\frac{n}{4(n-2)}} - \sqrt{\frac{n-1}{4(n-3)}}\right) \\ &\quad -\left(\frac{\sqrt{2}}{2} - \frac{2}{3}\right) \\ &< ABC(X_2^{n-5}), \end{aligned}$$

a contradiction.

Case 2 ($d(w) = 2$ for Each Vertex $w \in N(v_1)$): Let $N(v_1) = \{w_1, w_2, w_3\}$. Since $m = 2n-2$, by Lemma 2 we can deduce that there is another edge $x_1x_2 \in E_{3^+,3^+}$. With the result of Case 1, we can conclude that there is no neighbor of x_1 with degree two. If one assumes that $G' = G - x_1x_2 - v_1w_3 + v_1x_2 + w_3x_1$, it can be verified that $ABC(G) \leq ABC(G')$. As v_1 has a neighbor w_1 with $d(w_1) = 2$ and another neighbor x_2 with degree at least three. Applying further Case 1, we again obtain a contradiction. This assertion completes the proof. □

Lemma 5: If $G \in \mathcal{G}$, then $|E_{2,4}| = 0$.

Proof: Suppose on the contrary that there is an edge $w_1v_1 \in E_{2,4}$, we have w_1 has another neighbor $v_3 \in V_{4^+}$ by Lemmas 3 and 4.

Case 1: there are two vertices $v_2, v_4 \in N(v_1)$ with $\{v_2, v_4\} \subseteq V_{3^+}$.

Let $G' = G - \{w_1\}$, then we have $ABC(e|G) \leq ABC(e|G')$ for any $e \in E(G')$, $x_1 = d(v_2)$ and $x_2 = d(v_4)$ Then we have

$$ABC(w_1v_1|G) = ABC(w_1v_3|G) = \frac{\sqrt{2}}{2},$$

$$ABC(v_1v_2|G') = \sqrt{\frac{x_1+1}{3x_1}},$$
$$ABC(v_1v_4|G') = \sqrt{\frac{x_2+1}{3x_2}},$$
$$ABC(v_1v_2|G) = \sqrt{\frac{x_1+2}{4x_1}},$$

and

$$ABC(v_1v_4|G) = \sqrt{\frac{x_2+2}{4x_2}}.$$

Therefore, we have

$$\begin{aligned} ABC(G) &\leq ABC(G') + ABC(w_1v_1|G) \\ &\quad + ABC(w_1v_3|G) + ABC(v_1v_2|G) \\ &\quad + ABC(v_1v_4|G) - ABC(v_1v_2|G') \\ &\quad - ABC(v_1v_4|G') \\ &\leq ABC(G') + \sqrt{2} \\ &\quad + \sum_{i=1}^{2}\left(\sqrt{\frac{x_i+2}{4x_i}} - \sqrt{\frac{x_i+1}{3x_i}}\right) \\ &\leq ABC(G') + \sqrt{2} \\ &\quad + \sum_{i=1}^{2}\left(\sqrt{\frac{x_i+2}{4x_i}} - \sqrt{\frac{x_i+1}{3x_i}}\right)\Big|_{x_i=3} \\ &\leq ABC(G') + \sqrt{2} - 2\left(\frac{2}{3} - \sqrt{\frac{5}{12}}\right). \end{aligned}$$

Subcase 1.1 ($ABC(G') \leq ABC(X_1^{n-5})$): In this case, we have if $n \geq 10$, then

$$\begin{aligned} ABC(G) &\leq ABC(X_1^{n-5}) + \sqrt{2} - 2\left(\frac{2}{3} - \sqrt{\frac{5}{12}}\right) \\ &= ABC(X_1^{n-4}) \\ &\quad -4\left(\sqrt{\frac{n}{3(n-1)}} - \sqrt{\frac{n-1}{3(n-2)}}\right) \\ &\quad -\left(\frac{\sqrt{2n-4}}{n-1} - \frac{\sqrt{2n-6}}{n-2}\right) \\ &\quad -2\left(\frac{2}{3} - \sqrt{\frac{5}{12}}\right) \\ &< ABC(X_1^{n-4}), \end{aligned}$$

a contradiction.

Subcase 1.2 ($ABC(G') \leq ABC(X_2^{n-6})$): In this case, we have if $n \geq 10$, then

$$\begin{aligned} ABC(G) &\leq ABC(X_2^{n-6}) + \sqrt{2} - 2\left(\frac{2}{3} - \sqrt{\frac{5}{12}}\right) \\ &= ABC(X_2^{n-5}) \\ &\quad -4\left(\sqrt{\frac{n-1}{3(n-2)}} - \sqrt{\frac{n-2}{3(n-3)}}\right) \\ &\quad -2\left(\sqrt{\frac{n}{4(n-2)}} - \sqrt{\frac{n-1}{4(n-3)}}\right) \\ &\quad -2\left(\frac{2}{3} - \sqrt{\frac{5}{12}}\right) \\ &\leq ABC(X_2^{n-5}), \end{aligned}$$

a contradiction.

Case 2: there is exactly one vertex $v_2 \in N(v_1)$ with $v_2 \in V_{3^+}$.

Let $G' = G - \{w_1\}$, then we have $ABC(e|G) \leq ABC(e|G')$ for any $e \in E(G')$, $x = d(v_2)$ and so $x \geq 3$. Then consider the following cases.

Subase 2.1 ($x \geq 4$):

$$ABC(w_1v_1|G) = ABC(w_1v_3|G) = \frac{\sqrt{2}}{2},$$
$$ABC(v_1v_2|G') \geq \sqrt{\frac{x+1}{3x}},$$

and

$$ABC(v_1v_2|G) = \sqrt{\frac{x+2}{4x}}.$$

Therefore, we have

$$\begin{aligned} ABC(G) &\leq ABC(G') + ABC(w_1v_1|G) \\ &\quad + ABC(w_1v_3|G) + ABC(v_1v_2|G) \\ &\quad - ABC(v_1v_2|G') \\ &\leq ABC(G') + \sqrt{2} \\ &\quad + \left(\sqrt{\frac{x+2}{4x}} - \sqrt{\frac{x+1}{3x}}\right) \\ &\leq ABC(G') + \sqrt{2} \\ &\quad + \left(\sqrt{\frac{x+2}{4x}} - \sqrt{\frac{x+1}{3x}}\right)\Big|_{x=4} \\ &\leq ABC(G') + \sqrt{2} - \left(\sqrt{\frac{5}{12}} - \sqrt{\frac{6}{16}}\right). \end{aligned}$$

Subcase 2.1.1 ($ABC(G') \leq ABC(X_1^{n-5})$): In this case, we have if $n \geq 10$, then

$$\begin{aligned} ABC(G) &\leq ABC(X_1^{n-5}) + \sqrt{2} \\ &\quad -\left(\sqrt{\frac{5}{12}} - \sqrt{\frac{6}{16}}\right) \\ &= ABC(X_1^{n-4}) \\ &\quad -4\left(\sqrt{\frac{n}{3(n-1)}} - \sqrt{\frac{n-1}{3(n-2)}}\right) \\ &\quad -\left(\frac{\sqrt{2n-4}}{n-1} - \frac{\sqrt{2n-6}}{n-2}\right) \\ &\quad -\left(\sqrt{\frac{5}{12}} - \sqrt{\frac{6}{16}}\right) \\ &< ABC(X_1^{n-4}), \end{aligned}$$

a contradiction.

Subcase 2.1.2: $ABC(G') \leq ABC(X_2^{n-6})$.

In this case, we have if $n \geq 10$, then

$$\begin{aligned}ABC(G) &\leq ABC(X_2^{n-6}) + \sqrt{2} - \left(\sqrt{\frac{5}{12}} - \sqrt{\frac{6}{16}}\right)\\ &= ABC(X_2^{n-5})\\ &\quad -4\left(\sqrt{\frac{n-1}{3(n-2)}} - \sqrt{\frac{n-2}{3(n-3)}}\right)\\ &\quad -2\left(\sqrt{\frac{n}{4(n-2)}} - \sqrt{\frac{n-1}{4(n-3)}}\right)\\ &\quad -\left(\sqrt{\frac{5}{12}} - \sqrt{\frac{6}{16}}\right)\\ &\leq ABC(X_2^{n-5}),\end{aligned}$$

a contradiction.

Subcase 2.2 ($x = 3$): Since $d(v_4), d(v_5) \geq 3$, together with Lemma 4, we have $v_4v_1 \notin E(G)$. Now, let $N(v_2) = \{v_1, v_4, v_5\}$ and $G' = G - \{w_1\} - v_2v_4 + v_1v_4$. Since for $x \geq 3$,

$$2 \times \frac{\sqrt{2}}{2} + \sqrt{\frac{x+3}{5x}} \geq \sqrt{\frac{x+1}{3x}} + \sqrt{\frac{5}{12}} + \frac{2}{3},$$

we have $ABC(G') \geq ABC(G)$.

Now we can obtain a contradiction by similar argument to the proof of Case 1.

Case 3 ($d(w) = 2$ for Each Vertex $w \in N(v_1)$): Let $N(v_1) = \{w_1, w_2, w_3, w_4\}$. Since $m = 2n - 2$, by Lemma 2 we can deduce that there is another edge $x_1x_2 \in E_{3^+,3^+}$. It is sufficient to consider the following cases.

Subcase 3.1 ($x_1x_2 \in E_{3,3}$): By Lemma 4, we have $d(u) \geq 3$ for any $u \in N(x_i)(i = 1, 2)$. Let s_1 and s_2 be two of the neighbors of x_1, $y_1 = d(s_1)$, and $y_2 = d(s_2)$, we have $y_1 \geq 3, y_2 \geq 3$. Let $G' = G - x_1x_2 + v_1x_2$, now we have

$$\begin{aligned}ABC(G) &\leq ABC(G') - \sqrt{\frac{6}{15}} + \frac{2}{3} - \sqrt{2}\\ &\quad + \sqrt{\frac{y_1+1}{3y_1}} + \sqrt{\frac{y_2+1}{3y_2}}\\ &\leq ABC(G') - \sqrt{\frac{6}{15}} + \frac{2}{3} - \sqrt{2} + \frac{4}{3}\\ &< ABC(G'),\end{aligned}$$

a contradiction.

Subcase 3.2 ($x_1x_2 \in E_{3^+,4^+}$): Assume $G' = G - x_1x_2 - v_1w_4 + v_1x_1 + w_4x_2$ and it can be verified that $ABC(G) \leq ABC(G')$. But v_1 has a neighbor w_1 with $d(w_1) = 2$ and another neighbor x_1 with degree at least three. Applying now Case 1, we obtain a contradiction. This assertion completes the proof. □

By similar argument to the proof of Lemma 5, we can obtain Lemma 6.

Lemma 6: Let $G \in \mathcal{G}$ and G be an (n, m)-graph with $m = 2n - 2$, $\delta(G) \geq 2$ and G has the maximum ABC index.

i) If $k = 6$ and $|V_3| \geq 1$ or $k \leq 5$, then $|E_{2,5}| = 0$;

ii) If $n \geq 13$, $k = 5$ and $N(v)$ contains at least two vertices with degree at least three for each $v \in V_6$, then $|E_{2,6}| = 0$.

Lemma 7: If $G \in \mathcal{G}$, then G contains no induced $P_3 = w_1w_2w_3$ such that $d(w_1) = d(w_2) = 3$ and $d(w_3) \geq 3$.

Proof: Suppose on the contrary that G contains an induced $P_3 = w_1w_2w_3$ such that $d(w_1) = d(w_2) = 3$ and $d(w_3) \geq 3$. Let $G' = G - \{w_2\} + w_1w_3$, then G' is an $(n-1, 2n-4)$-graph.

Case 1 ($ABC(G') \leq ABC(X_1^{n-5})$): Since $n \geq 10$, we have

$$\begin{aligned}ABC(G) &\leq ABC(G') + \frac{4}{3}\\ &\leq ABC(X_1^{n-5}) + \frac{4}{3}\\ &\leq ABC(X_1^{n-4}) - \sqrt{2}\\ &\quad - 4\left(\sqrt{\frac{n}{3(n-1)}} - \sqrt{\frac{n-1}{3(n-2)}}\right)\\ &\quad - \left(\frac{\sqrt{2n-4}}{n-1} - \frac{\sqrt{2n-6}}{n-2}\right) + \frac{4}{3}\\ &< ABC(X_1^{n-4}),\end{aligned}$$

a contradiction.

Case 2 ($ABC(G') \leq ABC(X_2^{n-6})$): Since $n \geq 10$, we have

$$\begin{aligned}ABC(G) &\leq ABC(X_2^{n-6}) + \frac{4}{3}\\ &= ABC(X_2^{n-5}) - \sqrt{2}\\ &\quad - 4\left(\sqrt{\frac{n-1}{3(n-2)}} - \sqrt{\frac{n-2}{3(n-3)}}\right)\\ &\quad - 2\left(\sqrt{\frac{n}{4(n-2)}} - \sqrt{\frac{n-1}{4(n-3)}}\right) + \frac{4}{3}\\ &\leq ABC(X_2^{n-5}),\end{aligned}$$

a contradiction. This assertion completes the proof. □

By similar argument to the proof of Lemma 7, we have the following result and omit the proof.

Lemma 8: If $G \in \mathcal{G}$, then G contains no induced $P_3 = w_1w_2w_3$ such that $d(w_1) = 4$, $d(w_2) = 3$ and $d(w_3) = 4$.

Lemma 9: Let $G \in \mathcal{G}$ and $k \geq 6$. If $w_1w_2w_3$ is a triangle in $G[V_3]$, then there is no vertex $s \in V_{3^+} \setminus \{w_1, w_2, w_3\}$ such that $|N(s) \cap \{w_1, w_2, w_3\}| \geq 2$.

Proof: Otherwise, we may assume that there is a vertex $s \in V_{3^+} \setminus \{w_1, w_2, w_3\}$ such that $|N(s) \cap \{w_1, w_2, w_3\}| \geq 2$ and $sw_1, sw_3 \in E(G)$.

Now we claim that there is an edge $t_1t_2 \in E_{3^+,3^+} \setminus (E_s \cup \{w_1w_2, w_1w_3, w_2w_3\})$. Otherwise, $|E_{3^+,3^+}| \leq |E_s \cup \{w_1w_2, w_1w_3, w_2w_3\}| \leq 3 + k - 1 = k + 2$. By Lemma 2, we have $\ell_3 = 2k - 2 = |E_{3^+,3^+}| \leq k + 2$. Hence $k \leq 4$, a contradiction.

Now it is sufficient to consider the following two cases.

Case 1 ($w_1t_1 \notin E(G)$ and $w_1t_2 \notin E(G)$): In this case, $t_1, t_2 \notin \{s, w_1, w_2, w_3\}$, and we can deduce that $w_3t_1 \notin E(G)$ and $w_3t_2 \notin E(G)$. Let $G' = G - w_1w_3 - t_1t_2 + w_1t_1 + w_3t_2$,

$f(x,y)=\sqrt{\frac{x+y-2}{xy}}$ and we have

$$\begin{aligned}ABC(G) &\leq ABC(G')+ABC(w_1w_3|G)+ABC(t_1t_2|G)\\ &\quad -ABC(w_1t_1|G')-ABC(w_3t_2|G')\\ &\leq ABC(G')+f(3,3)+f(d(t_1),d(t_2))\\ &\quad -f(3,d(t_1))-f(3,d(t_2))\\ &< ABC(G'),\end{aligned}$$

a contradiction.

Case 2 ($w_1t_1 \notin E(G)$ and $w_1t_2 \in E(G)$): Since $d(w_1)=3$, we have $t_2 \in N(w_1)=\{s,w_2,w_3\}$. In this case, we have that t_2 cannot be any vertex in $\{s,w_3\}$. Hence, t_2 is exactly the vertex w_2. Now we claim that there is an edge $q_1q_2 \in E_{3^+,3^+}\setminus(E_s\cup E_{w_1}\cup E_{w_2}\cup E_{w_3})$. Otherwise, $|E_{3^+,3^+}|=|E_s\cup\{w_1w_2,w_1w_3,w_2w_3,w_2t_1\}|\leq 4+k-1=k+3$. By Lemma 2, we have $\ell_3=2k-2=|E_{3^+,3^+}|\leq k+3$. Hence $k\leq 5$, a contradiction. Now, since $d(w_1)=d(w_3)=3$, we can deduce that $N(w_i)\cap\{q_1,q_2\}=\emptyset$ for any $i\in\{1,3\}$. Let $G'=G-w_1w_3-q_1q_2+w_1q_1+w_3q_2, f(x,y)=\sqrt{\frac{x+y-2}{xy}}$ and we have

$$\begin{aligned}ABC(G) &\leq ABC(G')+ABC(w_1w_3|G)\\ &\quad +ABC(q_1q_2|G)-ABC(w_1q_1|G')\\ &\quad -ABC(w_3q_2|G')\\ &\leq ABC(G')+f(3,3)+f(d(q_1),d(q_2))\\ &\quad -f(3,d(q_1))-f(3,d(q_2))\\ &< ABC(G'),\end{aligned}$$

a contradiction. This assertion completes the proof. □

Lemma 10: Let $G\in\mathcal{G}$ and $k\geq 6$. Then $G[V_3]$ contains no triangle.

Proof: Suppose on the contrary that $G[V_3]$ contains a triangle $w_1w_2w_3$. Then, there is an edge $t_1t_2\in E_{3^+,3^+}\setminus(E_{w_1}\cup E_{w_2}\cup E_{w_3})$ and we have $|N(w_i)\cap\{t_1,t_2\}|\leq 1$ for any $i\in\{1,2,3\}$. Now it is sufficient to consider the following cases.

Case 1 ($w_1t_2\notin E(G)$ and $w_3t_1\notin E(G)$): Let $G'=G-w_1w_3-t_1t_2+w_1t_2+w_3t_1$, and $ABC(G)\leq ABC(G')$. Since $t_1t_2\in E_{3^+,3^+}\setminus(E_{w_1}\cup E_{w_2}\cup E_{w_3})$, we have $w_1\neq t_2$ and $w_3\neq t_1$. As $G'[V_3]$ has an induced $P_3=w_1w_2w_3$, we can obtain a contradiction by Lemma 7.

Case 2 ($w_1t_2\notin E(G)$ and $w_3t_1\in E(G)$): In this case, we have $w_1t_1\notin E(G)$ and $w_3t_2\notin E(G)$ by Lemma 9. Let $G'=G-w_1w_3-t_1t_2+w_1t_1+w_3t_2$, and we have $ABC(G)\leq ABC(G')$. As $G'[V_3]$ has an induced $P_3=w_1w_2w_3$, we can obtain a contradiction by Lemma 7. This assertion completes the proof. □

Lemma 11: Let $G\in\mathcal{G}$ and $k\geq 6$. If $w_1w_2w_3$ is a triangle such that $d(w_1)=d(w_2)=3$, $d(w_3)=4$ and another edge $t_1t_2\in E_{3^+,3^+}\setminus\{w_1w_2,w_1w_3,w_2w_3\}$, then it is impossible that $w_1t_2\notin E(G)$ and $w_3t_1\notin E(G)$ with $w_1\neq t_2$ and $w_3\neq t_1$.

Proof: Suppose on the contrary that G contains a triangle $P_3=w_1w_2w_3$ such that $d(w_1)=d(w_2)=3$ and $d(w_3)=4$. Then there is an edge $t_1t_2\in E_{3^+,3^+}\setminus\{w_1w_2,w_1w_3,w_2w_3\}$. If $d(t_2)\geq 4$, then let $G'=G-w_1w_3-t_1t_2+w_1t_2+w_3t_1$, and we have $ABC(G)\leq ABC(G')$. Then we can process G' applying Lemma 7, and obtain a contradiction.

If $d(t_2)=3$, then let $G'=G-\{w_2\}-t_1t_2+w_1t_2+w_3t_1$. Then G' is an $(n-1,2n-2)$-graph. we have $ABC(G)\leq ABC(G')+\frac{4}{3}-\frac{2}{3}-\sqrt{\frac{d(t_1)+2}{4d(t_1)}}-\sqrt{\frac{d(t_1)+1}{3d(t_1)}}+\sqrt{\frac{5}{12}}$. By similar argument to the proof of Lemma 7, we can obtain a contradiction. This assertion completes the proof. □

By similar argument to the proof of Lemma 9, we have obtained the following lemma and omit the proof.

Lemma 12: Let $G\in\mathcal{G}$ and $k\geq 6$. If $w_1w_2w_3$ is a triangle such that $d(w_1)=d(w_2)=3$ and $d(w_3)=4$, then there is no vertex $s\in V_{3^+}\setminus\{w_1,w_2,w_3\}$ such that $|N(s)\cap\{w_1,w_3\}|\geq 2$.

Lemma 13: Let $G\in\mathcal{G}$ and $k\geq 6$. Then there is no triangle $w_1w_2w_3$ such that $d(w_1)=d(w_2)=3$ and $d(w_3)=4$.

Proof: Suppose on the contrary that there is a triangle $w_1w_2w_3$ such that $d(w_1)=d(w_2)=3$ and $d(w_3)=4$. Consequently, there is an edge $t_1t_2\in E_{3^+,3^+}\setminus(E_{w_1}\cup E_{w_2}\cup E_{w_3})$. Then, we can conclude that $|N(w_i)\cap\{t_1,t_2\}|\leq 1$ for any $i\in\{1,3\}$. Otherwise, we can obtain a contradiction. Now it is sufficient to consider the following cases.

Case 1 ($w_1t_2\notin E(G)$ and $w_3t_1\notin E(G)$): Let $G'=G-w_1w_3-t_1t_2+w_1t_2+w_3t_1$, and we have $ABC(G)\leq ABC(G')$. Since $t_1t_2\in E_{3^+,3^+}\setminus(E_{w_1}\cup E_{w_2}\cup E_{w_3})$, we have $w_1\neq t_2$ and $w_3\neq t_1$. As G' has an induced $P_3=w_1w_2w_3$ with $d(w_1)=d(w_2)=2$ and $d(w_3)=4$, we obtain a contradiction by Lemma 11.

Case 2 ($w_1t_2\notin E(G)$ and $w_3t_1\in E(G)$): In this case, by Lemma 12, we have $w_1t_1\notin E(G)$. Then we have $w_3t_2\in E(G)$. Otherwise, $w_1t_1\notin E(G)$, $w_3t_2\notin E(G)$, $w_1\notin t_1$ and $w_3\notin t_2$, contradicting with Lemma 11.

Now we claim that there is an edge $q_1q_2\in E_{3^+,3^+}\setminus(E_{w_1}\cup E_{w_2}\cup E_{w_3}\cup\{t_1t_2\})$. Then, $|N(w_1)\cap\{q_1,q_2\}|\leq 1$ since $d(w_1)=3$. We may assume w.l.o.g. that $w_1q_2\notin E(G)$, then by Lemma 11 we have $w_3q_1\in E(G)$. Hence $w_3q_2\notin E(G)$. Otherwise, we have $q_1q_2=t_1t_2$, a contradiction. Now by Lemma 11 with q_1q_2 playing the role of t_1t_2, we obtain a contradiction. This assertion completes the proof. □

Lemma 14: Let $G\in\mathcal{G}$ and $k\geq 6$. Then $k\leq 9$.

Proof: Let

$$M_1=\bigcup_{e\in E_{3,3}}N'(e),$$
$$M_2=E_{3^+,3^+}\setminus(E_{3,3}\cup M_1)$$

then we have

$$\sum_{e\in E_{3,3}}ABC(e)=\frac{2|E_{3,3}|}{3},$$

$$\sum_{e\in M_1}ABC(e)\leq 4\sqrt{\frac{6}{15}}|E_{3,3}|,$$

$$\sum_{e\in M_2}ABC(e)\leq(2k-2-5|E_{3,3}|)\sqrt{\frac{5}{12}},$$

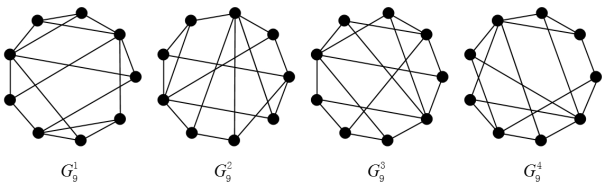

FIGURE 2. The graphs used in the proof of Lemma 15.

$$\sum_{e\in E_{2,3^+}} ABC(e) = (n-k)\sqrt{2},$$

and

$$\begin{aligned} ABC(G) &= \sum_{e\in E_{3,3}} ABC(e) + \sum_{e\in M_1} ABC(e) \\ &\quad + \sum_{e\in M_2} ABC(e) + \sum_{e\in E_{2,3^+}} ABC(e) \\ &\le \frac{2|E_{3,3}|}{3} + 4\sqrt{\frac{6}{15}}|E_{3,3}| \\ &\quad +(2k-2-5|E_{3,3}|)\sqrt{\frac{5}{12}} + (n-k)\sqrt{2} \\ &\le (2k-2)\sqrt{\frac{5}{12}} + (n-k)\sqrt{2}. \end{aligned}$$

By Lemma 1, we have $ABC(X_2^{n-5}) = 4\sqrt{\frac{n-1}{3(n-2)}}+2\sqrt{\frac{n}{4(n-2)}}+(n-5)\sqrt{2}+2\sqrt{\frac{5}{12}}$. It can be verified that if $k \ge 10$, $ABC(G) < ABC(X_2^{n-5})$, a contradiction. □

In order to prove Lemma 15, we give the following definitions.

For a graph G, $a \in \mathbb{N}$ and $S \subseteq \mathbb{N}$, we define a function $d' : V(G) \to \mathbb{N}$ with

$$d'(v) = \begin{cases} a, & d(v) \in S, \\ d(v), & d(v) \notin S, \end{cases}$$

and

$$ABC'_{S\to a}(G) = \sum_{uv\in E(G)} \sqrt{\frac{d'(u)+d'(v)-2}{d'(u)d'(v)}}.$$

Lemma 15: Let $G \in \mathcal{G}$ and $k \ge 6$. Then $k \ne 9$.

Proof: Suppose on the contrary that $k = |V_{3^+}| = 9$, then since $|E_{2,3}| = 0$ and $|E_{2,4}| = 0$ we have $\sum_{e\in E_{3^+,3^+}} ABC(e) \le ABC'_{\{1,2\}\to 5}(G[V_{3^+}])$. By an exhaustive search in the set of (9, 16)-graphs, we obtain that $ABC'_{\{1,2\}\to 5}(G[V_{3^+}]) \le ABC'_{\{1,2\}\to 5}(H) \approx 10.2398775511417$, where H is one of the graphs depicted in Figure 2.

Since $n \ge 10$, we have

$$\begin{aligned} &ABC(G) - ABC(X_2^{n-5}) \\ &\le \sum_{e\in E_{3^+,3^+}} ABC(e) + \sum_{e\in E_{2,3^+}} ABC(e) - ABC(X_2^{n-5}) \\ &\le ABC'_{\{1,2\}\to 5}(G[V_{3^+}]) + (2n-2-16)\sqrt{\frac{1}{2}} \\ &\quad -4\sqrt{\frac{n-1}{3(n-2)}} - 2\sqrt{\frac{n}{4(n-2)}} \\ &\quad -(n-5)\sqrt{2} - 2\sqrt{\frac{5}{12}} \\ &< 10.24 + (2n-2-16)\sqrt{\frac{1}{2}} \\ &\quad -4\sqrt{\frac{n-1}{3(n-2)}} - 2\sqrt{\frac{n}{4(n-2)}} \\ &\quad -(n-5)\sqrt{2} - 2\sqrt{\frac{5}{12}} \\ &< 0, \end{aligned}$$

which is a contradiction to the initial assumption. □

Lemma 16: Let $G \in \mathcal{G}$ and $k \ge 6$. Then $k \ne 8$.

Proof: Let

$$M_1 = \bigcup_{e\in E_{3,3}} N'(e),$$
$$M_2 = E_{3^+,3^+} \setminus (E_{3,3} \cup M_1).$$

Suppose on the contrary that $k = |V_{3^+}| = 8$, we have

Claim 2: $|V_3| \ge 4$.

Proof: Suppose on the contrary that $|V_3| \le 3$, we consider the following two cases.

Case 1: there is an edge $w_1v_1 \in E_{3,3}$.

In this case, by Lemmas 7,10 and 13,we have

$$\sum_{e\in N'(w_1v_1)} ABC(e) \le 4\sqrt{\frac{3+5-2}{3\times 5}}.$$

Since $|V_3| \le 3$, we have $|E_{3,4^+}| \le 3$. Since $|E_{3^+,3^+}| = 2\times 8-2 = 14$, we have $|E_{3,4^+} \setminus N'(w_1v_1)| + |E_{4^+,4^+}| = 9$. Since $d(w_1) = d(v_1) = 3$, together with Lemmas 7,10 and 13, we have

$$\sum_{e\in J} ABC(e) + \sum_{e\in E_{4^+,4^+}} ABC(e) \le 3\sqrt{\frac{5}{12}} + 6\sqrt{\frac{6}{16}},$$

where $J = E_{3,4^+} \setminus N'(w_1v_1)$, and

$$\sum_{e\in E_{2,3^+}} ABC(e) \le (n-8)\sqrt{2},$$

and thus

$$\begin{aligned} ABC(G) &\le ABC(w_1v_1) + \sum_{e\in N'(w_1v_1)} ABC(e) \\ &\quad + \sum_{e\in E_{3,4}\setminus N'(w_1v_1)} ABC(e) \\ &\quad + \sum_{e\in E_{4^+,4^+}} ABC(e) + \sum_{e\in E_{2,3^+}} ABC(e) \\ &\le \frac{2}{3} + 4\sqrt{\frac{6}{15}} + 3\sqrt{\frac{5}{12}} + 6\sqrt{\frac{6}{16}} + (n-8)\sqrt{2}. \end{aligned}$$

Since $n \geq 10$, we have

$$ABC(G) - ABC(X_2^{n-5}) < 0,$$

a contradiction.

Case 2 ($|E_{3,3}| = 0$): We first prove the following claim:

$$|V_3| + |V_4| \leq 6. \quad (6)$$

Otherwise, since $k = 8$ and $|E_{2,2}| = |E_{2,3}| = |E_{2,4}| = 0$, there is at most one vertex $u \in V_{4^+}$. Since any vertex with degree two is only adjacent to u, we conclude that such a graph does not exist, which is a contradiction.

Then we claim that $|E_{3,4}| \leq 6$. Otherwise, we assume that $|E_{3,4}| \geq 7$, and consequently, there are at least three vertices with degree three. Since $|V_3| \leq 3$, we have $|V_3| = 3$. From $|E_{3,4}| \geq 7$ and $|V_3| + |V_4| \leq 6$, we have $|V_4| \leq 3$. Further, we also have a vertex $v \in V_3$ where each vertex in $N(v)$ has degree four whereby $|V_4| = 3$. By Lemma 8, we conclude that the vertices in $N(v)$ are pairwise adjacent. Now it can be checked that $|E_{3,4}| \leq 6$, contradicting with the assumption $|E_{3,4}| \geq 7$.

Then we have $|E_{3,5^+}| + |E_{3,4}| \leq 9$, and so

$$\begin{aligned} ABC(G) \leq & \sum_{e \in E_{3,4^+}} ABC(e) + \sum_{e \in E_{4^+,4^+}} ABC(e) \\ & + \sum_{e \in E_{2,3^+}} ABC(e) \\ \leq & |E_{3,4}|\sqrt{\frac{5}{12}} + |E_{3,5^+}|\sqrt{\frac{6}{15}} \\ & + (14 - |E_{3,5^+}| - |E_{3,4}|)\sqrt{\frac{6}{16}} \\ & + (n-8)\sqrt{2} \\ \leq & 6\sqrt{\frac{5}{12}} + 3\sqrt{\frac{6}{15}} + 5\sqrt{\frac{6}{16}} + (n-8)\sqrt{2}. \end{aligned}$$

Since $n \geq 10$, we have

$$ABC(G) - ABC(X_2^{n-5}) < 0,$$

a contradiction. □

Claim 3: $|V_3| \neq 4$.

Proof: Suppose on the contrary that $|V_3| = 4$, we then have $|E_{3,3}| \leq 2$.

If $|E_{3,3}| = 2$, then $G[V_3]$ is a matching of four vertices by Lemma 8. By Lemma 7 and Lemma 13, we have $e' \notin E_{3,4}$ for each $e' \in N'(e)$ for any $e \in E_{3,3}$. Hence $|E_{3,4}| = 0$, and thus

$$\begin{aligned} ABC(G) \leq & \sum_{e \in E_{3,3}} ABC(e) + \sum_{e \in M_1} ABC(e) \\ & + \sum_{e \in E_{4^+,4^+}} ABC(e) + \sum_{e \in E_{2,3^+}} ABC(e) \\ \leq & \frac{4}{3} + 8\sqrt{\frac{6}{15}} + 4\sqrt{\frac{6}{16}} + (n-8)\sqrt{2}. \end{aligned}$$

Since $n \geq 10$, we have

$$ABC(G) - ABC(X_2^{n-5}) < 0,$$

a contradiction.

If $|E_{3,3}| = 1$, we can deduce that $|V_3|+|V_4| \leq 6$ by similar argument to the proof of Case 2 (see Eq. (6)). Since $|V_3| = 4$, we have $|V_4| \leq 2$. Hence $|E_{3,4}| \leq 4$ and $|E_{4,4}| \leq 1$. Then we have

$$\sum_{e \in (E_{3,4^+} \setminus M_1)} ABC(e) \leq 4\sqrt{\frac{5}{12}} + 2\sqrt{\frac{6}{15}},$$

$$\sum_{e \in E_{4^+,4^+}} ABC(e) \leq \sqrt{\frac{6}{16}} + 2\sqrt{\frac{7}{20}},$$

and thus

$$\begin{aligned} ABC(G) \leq & \sum_{e \in E_{3,3}} ABC(e) \\ & + \sum_{e \in M_1} ABC(e) + \sum_{e \in (E_{3,4^+} \setminus M_1)} ABC(e) \\ & + \sum_{e \in E_{4^+,4^+}} ABC(e) + \sum_{e \in E_{2,3^+}} ABC(e) \\ \leq & \frac{2}{3} + 4\sqrt{\frac{6}{15}} + 4\sqrt{\frac{5}{12}} + 2\sqrt{\frac{6}{15}} + \sqrt{\frac{6}{16}} \\ & + 2\sqrt{\frac{7}{20}} + (n-8)\sqrt{2}. \end{aligned}$$

Since $n \geq 10$, we have

$$ABC(G) - ABC(X_2^{n-5}) < 0,$$

a contradiction.

If $|E_{3,3}| = 0$, we can deduce that $|V_3| + |V_4| \leq 6$ by similar argument to the proof of Case 2 (see Eq. (6)) and thus $|V_4| \leq 2$.

Now we claim that $|V_4| = 2$. (Otherwise, we have $|V_4| \leq 1$). Now we have

$$\begin{aligned} ABC(G) \leq & \sum_{e \in E_{3,4^+}} ABC(e) + \sum_{e \in E_{4^+,4^+}} ABC(e) \\ & + \sum_{e \in E_{2,3^+}} ABC(e) \\ \leq & 4\sqrt{\frac{5}{12}} + 8\sqrt{\frac{6}{15}} + 2\sqrt{\frac{7}{20}} + (n-8)\sqrt{2}. \end{aligned}$$

Since $n \geq 10$, we have $ABC(G) - ABC(X_2^{n-5}) < 0$, a contradiction.

Now we have both $G[V_{3^+}]$ and G contains at least four vertices t_1, t_2, t_3, t_4 with degree three and two vertices s_1, s_2 with degree four. Further, $G[V_{3^+}]$ contains another two vertices w_1, w_2 and each vertex with degree two is adjacent to w_1 and w_2. By computer search, we obtain that if $|V_3'| = 4$ there is a total of four graphs for G and eight possibilities with different w_1 and w_2, which are presented in Figure 3; and if $|V_3'| = 5$ there is a total of seven graphs for G and seven possibilities with different w_1 and w_2, which are presented in Figure 4.

We can verify that $ABC(G) < ABC(X_2^{n-5})$ for each graph $G = T(G_8^i, w_1, w_2, n-8)$ ($i \in \{1, 2, \cdots, 15\}$), a contradiction. □

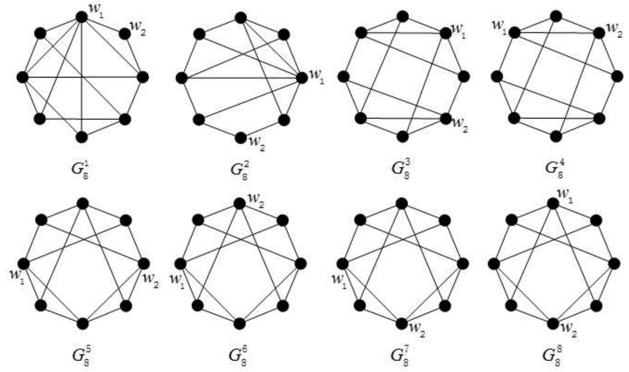

FIGURE 3. The graphs used in the proof of Claim 2 if $|E_{3,3}| = 0$ and $|V_3'| = 4$.

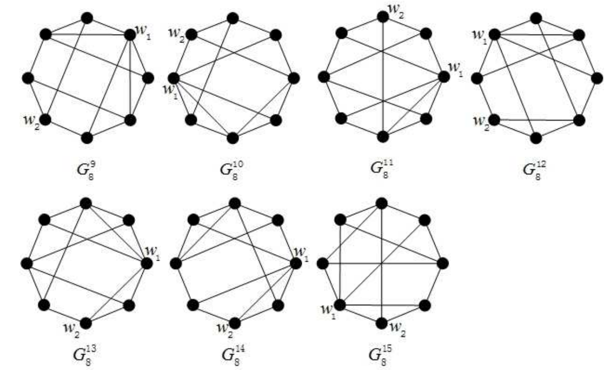

FIGURE 4. The graphs used in the proof of Claim 2 if $|E_{3,3}| = 0$ and $|V_3'| = 5$.

Claim 4: $|V_3| \neq 5$.

Proof: Suppose on the contrary that $|V_3| = 5$, similar to the proof of Claim 2 we have $|E_{3,3}| \leq 2$.

If $|E_{3,3}| = 0$, then $G[V_3]$ is an independent set. If $G[V_{3+}]$ has exactly five vertices with degree three, then $G[V_{3+}]$ has 8 vertices, 14 edges, 5 vertices with degree three and contains no edge in $E_{3,3}$. However, such a graph does not exist. We can also deduce that it is impossible for $G[V_{3+}]$ to have exactly p vertices with degree three for each $p \in \{6, 7, 8\}$. Hence, we obtain a contradiction.

If $|E_{3,3}| = 1$, we consider the following two cases.

Case 1 ($|V_3'| = 5$): In this case, we have $|E_{3,3}'| = 1$. By computer search, we find only one (8,14)-graph (depicted as G_8^{16} in Figure 5) satisfying the condition $|V_3'| = 5$ and $|E_{3,3}'| = 1$. For the unique edge $u_3u_4 \in E_{3,3}'$, it can be seen that $N(u_3) \neq N(u_4)$. On the other hand, we have $xz \in E(G)$ for any $P_3 = xyz$ with $d(x) = d(y) = 3$ and $d(z) \geq 3$ By Lemma 7. By applying $\{x, y\} = \{u_3, u_4\}$, we have $N(u_3) = N(u_4)$, a contradiction.

Case 2 ($|V_3'| = 6$): In this case, we have $|E_{3,3}'| \leq 4$. By computer search, we find four (8,14)-graphs satisfying the condition $|V_3'| = 6$ and $|E_{3,3}'| \leq 4$. By observing these graphs, we find each of them has $|E_{3,3}'| = 4$. It follows that there is a vertex $x \in V_3'$ adjacent to other three vertices in V_3' with degree three. In the set of above four graphs, there is only one graph satisfying this condition which is depicted as G_8^{17} in Figure 5. By observing the graph G_8^{17}, it can be seen that $V_3' = \{u_1, u_3, u_4, u_6, u_7, u_8\}$ and $V_5' = \{u_2, u_5\}$. Since $|V_3| = 5$ and $|V_{3+}| = 8$, we have $|V_{4+}| = 3$. Now we may assume w.l.o.g. that $|V_4^+| = \{t_1, t_2, t_3\}$, $d(t_1) = x$, $d(t_2) = y$, and $d(t_3) = z$ with $x \leq y \leq z$. Note that $V_{4+} \supseteq \{u_2, u_5\}$, $|E_{2,3}| = 0$, $|E_{2,4}| = 0$ and $V_5' = \{u_2, u_5\}$, we have $5 \leq x \leq y \leq z$ and $x+y+z = 2n-3$. That is to say, G is a graph obtained by adding $n-8$ vertices with degree two to G_8^{17} such that each vertex with degree two is adjacent to vertices in $\{t_1, t_2, t_3\}$.

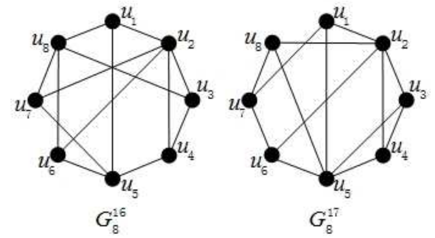

FIGURE 5. The graphs used in the proof of Claim 2 if $|E_{3,3}| = 1$.

Let $c = 2n - 3$,

$$f(x, y) = \frac{2}{3} + 5\sqrt{\frac{x+1}{3x}} + 5\sqrt{\frac{y+1}{3y}} + 3\sqrt{\frac{2n-3-x-y+1}{3(2n-3-x-y)}} + (n-8)\sqrt{2},$$

then we have

$$\begin{aligned}\frac{\partial f(x,y)}{\partial x} &= \frac{\sqrt{3}}{2(c-x-y)^2\sqrt{\frac{c-x-y+1}{c-x-y}}} - \frac{5}{2\sqrt{3}x^2\sqrt{\frac{x+1}{x}}} \\ &< \frac{\sqrt{3}}{2}\left(\frac{1}{z^2\sqrt{\frac{z+1}{z}}} - \frac{1}{x^2\sqrt{\frac{x+1}{x}}}\right) \\ &\leq 0.\end{aligned}$$

Similarly, we have $\frac{\partial f(x,y)}{\partial y} < 0$. Since $n \geq 10$, we have

$$\begin{aligned}ABC(G) &\leq f(x, y) \leq f(5, 5) \\ &\leq \frac{2}{3} + 10\sqrt{\frac{6}{15}} + 3\sqrt{\frac{2n-12}{3(2n-13)}} + (n-8)\sqrt{2} \\ &< ABC(X_2^{n-5}),\end{aligned}$$

which is a contradiction to the initial assumption.

If $|E_{3,3}| = 2$, then $G[V_3]$ is a matching of four vertices by Lemmas 7 and 10. We may assume without loss of generality that $V_{3+} = \{u_1, u_2, \cdots, u_8\}$ such that $E_{3,3} = \{u_1u_2, u_3u_4\}$, $d(u_5) = 3$ and $\{d(u_6), d(u_7), d(u_8)\} = \{x, y, z\}$ with $x \leq y \leq z$. Then we have $x + y + z = 2n - 3$.

Let $c = 2n - 3$ and

$$f(x, y) = \frac{4}{3} + 5\sqrt{\frac{x+1}{x}} + 5\sqrt{\frac{y+1}{y}} + \sqrt{\frac{c-x-y+1}{3(c-x-y)}} + \sqrt{\frac{x+y-2}{xy}} + (n-8)\sqrt{2}.$$

Similarly, we have $\frac{\partial f(x,y)}{\partial x} < 0$ and $\frac{\partial f(x,y)}{\partial y} < 0$. Since $|V_3| = 5$, we have $4 \leq x \leq y \leq z$. Therefore, we have if $n \geq 10$,

$$\begin{aligned} ABC(G) &\leq f(x,y) \leq f(4,4) \\ &\leq \frac{4}{3} + 10\sqrt{\frac{5}{12}} + \sqrt{\frac{2n-10}{6n-33}} \\ &\quad + \sqrt{\frac{6}{16}} + (n-8)\sqrt{2} \\ &< ABC(X_2^{n-5}), \end{aligned}$$

a contradiction. □

Claim 5: $|V_3| \neq 6$.

Proof: Suppose on the contrary that $|V_3| = 6$. Then we may assume without loss of generality that $G[V_{3+}] = \{w_1, w_2, \cdots, w_6, t_1, t_2\}$ where $d(w_i) = 3$ for each $i \in \{1, 2, \cdots, 6\}$ such that $N(v) = \{t_1, t_2\}$ each vertex v with degree two. If $|V_3'| = 6$, according to Lemma 7, $G[V_3]$ must be a matching. It can be verified that such a graph does not exist, a contradiction. If $|V_3'| = 7$, then $|E_{3,3}'| = 7$ since $|E(G[V_{3+}])| = 14$, we have $d_{G[V_{3+}]}(u_8) = 7$. Since $|E_{3,3}| \leq 2$, we have $|E_{3,3}'| \leq 5$, a contradiction. □

Claim 6: $|V_3| \neq 7$.

Proof: Suppose on the contrary that $|V_3| = 7$, then the vertex with degree two can not connect to any other vertices since $|E_{2,3}| = |E_{2,4}| = 0$, a contradiction. □

From the results of Claims 2–6, the claim of Lemma 16 follows. □

Lemma 17: Let $G \in \mathcal{G}$ and G be an (n,m)-graph, $k \geq 6$, $m = 2n-2$, $\delta(G) \geq 2$ and G has the maximum ABC index. Then $k \neq 7$.

Proof: Suppose on the contrary that $k = 7$, the proof is similar to that of Lemma 16. So we omit the detailed proof but give outline of the proof.

First, we need to claim that

$$|V_3| + |V_4| \leq 5, \tag{7}$$

then discuss the cases by different values of $|V_3|$.

If $|V_3| = 0$, we have $ABC(G) \leq 12\sqrt{\frac{6}{16}} + (n-7)\sqrt{2}$, and obtain that $ABC(G) < ABC(X_2^{n-5})$, which is a contradiction.

If $|V_3| = 1$, then $|V_4| \leq 4$ by Eq. (7). Then we can obtain that $|E_{3,4}| \leq 3$ and $|E_{4,4}| \leq \binom{4}{2} = 6$. Now we have $ABC(G) \leq 3\sqrt{\frac{5}{12}} + 6\sqrt{\frac{6}{16}} + 3\sqrt{\frac{7}{20}} + (n-7)\sqrt{2}$, and obtain that $ABC(G) < ABC(X_2^{n-5})$, which is a contradiction.

If $|V_3| = 2$, then $|V_4| \leq 3$ by Eq. (7). If $|E_{3,3}| = 1$, we have $|E_{3,4}| = 0$ and $|E_{4,4}| \leq 3$. Now we have $ABC(G) \leq \frac{2}{3} + 4\sqrt{\frac{6}{15}} + 3\sqrt{\frac{6}{16}} + 4\sqrt{\frac{7}{20}} + (n-7)\sqrt{2}$, and obtain that $ABC(G) < ABC(X_2^{n-5})$, which is a contradiction. If $|E_{3,3}| = 0$, we have $|V_4| \geq 3$ and thus $|V_4| = 3$. In this case, we can obtain a contradiction by similar argument to the proof of Claim 3.

If $|V_3| = 3$, then $|V_4| \leq 1$ by Eq. (7). We can process the cases $|V_3| \in \{3, 4\}$ by using similar approach to Claim 4.

If $|V_3| = 5$, the G is a graph such that each vertex with degree 2 is adjacent to two common vertices. We can process this case by using the approach used in the proof of Claim 3 in the case $|E_{3,3}| = 0$ and $|V_3'| = 4$. □

In order to prove Lemma 18, we can start with $|V_3| + |V_4| \leq 4$ and discuss the cases $|V_3|$. The proof is also similar and we also omit it.

Lemma 18: Let $G \in \mathcal{G}$ and G be an (n,m)-graph, $m = 2n-2$, $\delta(G) \geq 2$ and G has the maximum ABC index. Then $k \neq 6$.

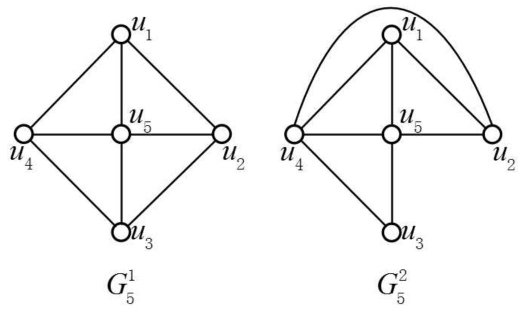

FIGURE 6. The graphs used in the proof of Lemma 19.

Lemma 19: Let $G \in \mathcal{G}$ and G be an (n,m)-graph, $n \geq 13$, $m = 2n-2$, $\delta(G) \geq 2$ and G has the maximum ABC index. If $k = 5$, then $G \cong X_2^{n-5}$.

Proof: We first assume on the contrary that $G \ncong X_2^{n-5}$.

Since $m = 2n-2$, we have $G[V_{3+}]$ is isomorphic to one of the graphs (G_5^1 and G_5^2) depicted in Figure 6. It is clear that G_5^1 or G_5^2 has no pendent vertices and $N_{G[V_{3+}]}(v)$ contains at least two vertices with degree at least two for each $v \in V_3'$. By Lemma 6 (ii), we have $|E_{2,6}| = 0$, and thus G contains no vertex with degree 6.

Since $|E_{2,5}| = 0$ by Lemma 6, we have G contains no vertex with degree 5, and

Claim 7: $|V_3 \cup V_4| \geq 2$.

Proof: Otherwise, we have $|V_3| = 0$ or $|V_4| = 0$. If $|V_4| = 0$, we have

$$\begin{aligned} ABC(G) &\leq \sum_{e \in E_{3,6+}} ABC(e) + \sum_{e \in E_{6+,6+}} ABC(e) \\ &\quad + \sum_{e \in E_{2,3+}} ABC(e) \\ &\leq 3\sqrt{\frac{7}{18}} + 5\sqrt{\frac{10}{36}} + (n-5)\sqrt{2} \\ &< ABC(X_2^{n-5}), \end{aligned}$$

a contradiction.

If $|V_3| = 0$, we have

$$\begin{aligned} ABC(G) &\leq \sum_{e \in E_{4,6+}} ABC(e) + \sum_{e \in E_{6+,6+}} ABC(e) \\ &\quad + \sum_{e \in E_{2,3+}} ABC(e) \\ &\leq 4\sqrt{\frac{7}{18}} + 4\sqrt{\frac{10}{36}} + (n-5)\sqrt{2} \\ &< ABC(X_2^{n-5}), \end{aligned}$$

a contradiction. □

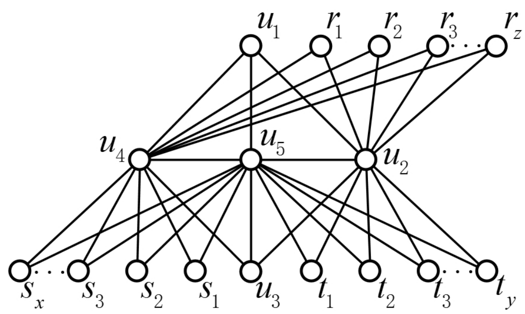

FIGURE 7. The graph $G^*(x, y, z)$.

Now we have

Claim 8: One of the following three cases holds.

1) $|V_3| = 2$ and $|E_{3,3}| = 0$;
2) $|V_3| = |V_4| = 1$ and $|E_{3,4}| = 0$;
3) $|V_3 \cup V_4| \geq 3$.

Proof: If $|V_3 \cup V_4| \leq 2$, then $|V_3 \cup V_4| = 2$ by Claim 7. If $|V_3| = 2$ and $|V_4| = 0$, then we have $|E_{3,3}| = 0$. Otherwise, there is at least an edge in $E_{3,3}$ and we have

$$\begin{aligned} ABC(G) \leq & \sum_{e\in E_{3,3}} ABC(e) + \sum_{e \in E_{3,7+}} ABC(e) \\ & + \sum_{e\in E_{7+,7+}} ABC(e) + \sum_{e\in E_{2,3+}} ABC(e) \\ & \leq \frac{2}{3} + 4\sqrt{\frac{8}{21}} + 3\sqrt{\frac{12}{49}} + (n-5)\sqrt{2} \\ & < ABC(X_2^{n-5}), \end{aligned}$$

a contradiction.

If $|V_3| = 1$ and $|V_4| = 1$, then we have $|E_{3,4}| = 0$ by similar argument to the proof of the case $|V_3| = 2$ and $|V_4| = 0$.

Similarly, we have that it is impossible if $|V_3| = 0$ and $|V_4| = 2$. $\square$

Case 1 ($|V_3| = 2$, $|V_4| = 0$ and $|E_{3,3}| = 0$): Now, we define some graphs as follows. Let G_5^1 be the left side graph depicted in Figure 5. For nonnegative integer x, y, z, we define a graph $G^*(x, y, z)$ by $V(G^*(x, y, z)) = V(G_5^1) \cup \{s_1, s_2, \ldots, s_x\} \cup \{t_1, t_2, \ldots, t_y\} \cup \{r_1, r_2, \ldots, r_z\}$, and $E(G^*(x, y, z)) = E(G_5^1) \cup \{s_1u_4, s_2u_4, \ldots, s_xu_4\} \cup \{s_1u_5, s_2u_5, \ldots, s_xu_5\} \cup \{t_1u_5, t_2u_5, \ldots, t_yu_5\} \cup \{t_1u_2, t_2u_2, \ldots, t_yu_2\} \cup \{r_1u_4, r_2u_4, \ldots, r_zu_4\} \cup \{r_1u_2, r_2u_2, \ldots, r_zu_2\}$. That is to say, $G^*(x, y, z)$ is obtained from G_5^1 by adding x vertices of degree two adjacent to both u_4 and u_5, adding y vertices of degree two adjacent to both u_5 and u_2 and adding z vertices of degree two adjacent to both u_4 and u_2 (see Figure 7).

Let $G_1 = G^*(x_1, y_1, z_1)$ and $G_2 = G^*(x_2, y_2, z_2)$ with $x_1 + y_1 + z_1 = x_2 + y_2 + z_2 = n - 5$. By symmetry, we assume $x_2 \geq y_2$. Then we have

Claim 9: If $z_1 = z_2$ and $x_1 = y_1$, then $ABC(G_1) \geq ABC(G_2)$.

Proof: Let $f(x, y) = 2\sqrt{\frac{4+x}{3(x+3)}} + 2\sqrt{\frac{4+y}{3(y+3)}} + \sqrt{\frac{1+x+t}{(3+x)t}} + \sqrt{\frac{1+y+t}{(3+y)t}}$. For any constant $c' \geq x$, we have that $f(x, c' - x)$ is monotonically decreasing with x on $[\frac{c'}{2}, +\infty)$.

Let $E' = \{u_4u_5, u_1u_4, u_3u_4, u_2u_5, u_1u_2, u_2u_3\}$, $t = d(u_5|G_1)$ and $c' = n-5-z_1$. Note that $d(u_5|G_2) = d(u_5|G_1)$, we have

$$\begin{aligned} & ABC(G_1) - ABC(G_2) \\ & = \sum_{e\in E'} (ABC(e|G_1) - ABC(e|G_2)) \\ & = 2\sqrt{\frac{4+x_1}{3(x_1+3)}} + 2\sqrt{\frac{4+y_1}{3(y_1+3)}} + \sqrt{\frac{1+x_1+t}{(3+x_1)t}} \\ & + \sqrt{\frac{1+y_1+t}{(3+y_1)t}} - 2\sqrt{\frac{4+x_2}{3(x_2+3)}} - 2\sqrt{\frac{4+y_2}{3(y_2+3)}} \\ & - \sqrt{\frac{1+x_2+t}{(3+x_2)t}} - \sqrt{\frac{1+y_2+t}{(3+y_2)t}} \\ & = f(x_1, y_1) - f(x_2, y_2) \\ & = f(x_1, c' - x_1) - f(x_2, c - x_2). \end{aligned}$$

Since $z_1 = z_2$ and $x_1 = y_1$, we have $x_2 \geq x_1$ and so $ABC(G_1) - ABC(G_2) \geq 0$. $\square$

By Claim 9, we have

$$\begin{aligned} & ABC(G^*(x, y, z))) \\ & \leq f\left(\frac{n-5-z}{2}, \frac{n-5-z}{2}\right) \\ & +2\sqrt{\frac{n-z}{3(n-1-z)}} + (n-5)\sqrt{2} \end{aligned}$$

It can be verified that $z = n - 5$ if and only if the function $f\left(\frac{n-5-z}{2}, \frac{n-5-z}{2}\right) + 2\sqrt{\frac{n-z}{3(n-1-z)}} + (n-5)\sqrt{2}$ reaches the maximum value. Therefore, if $ABC(G^*(x, y, z)))$ reaches the maximum value, we have $G \cong X_2^{n-5}$, contradicting with the assumption of G.

Case 2 ($|V_3| = |V_4| = 1$ and $|E_{3,4}| = 0$): By observing two graphs G_5^1 and G_5^2 in Figure 6, it can be easily inferred that the case is impossible.

Case 3 ($|V_3 \cup V_4| \geq 3$): In this case, G is a graph obtained by adding $n - 5$ vertices with degree two to two vertices in G_5^1 or G_5^2. We can obtain the desired result by using similar argument to the proof of Claim 3. $\square$

Lemma 20: Let G be an (n, m)-graph, $n \geq 10$, $m = 2n-2$, $\delta(G) \geq 2$ and G has the maximum ABC index. If $k = 4$, then $G \cong X_1^{n-4}$.

Proof: We first assume on the contrary that $G \ncong X_1^{n-4}$.

Since $|E_{2,4}| = |E_{2,5}| = 0$, we have $|V_4| = |V_5| = 0$ and G contains no vertex with degree 4 or 5. Then we have

Claim 10: $|V_3| \geq 1$.

Proof: Otherwise, we have

$$ABC(G) \leq \sum_{e \in E_{6^+,6^+}} ABC(e) + \sum_{e \in E_{2,3^+}} ABC(e) \leq 6\sqrt{\frac{10}{36}} + (n-4)\sqrt{2} < ABC(X_1^{n-4}),$$

a contradiction. □

Since $m = 2n-2$, we have $G[V_{3^+}] \cong K_4$. By Claim 10, $G \cong H(x, y, z)$ for some x, y, z with $x + y + z = n - 4$. Let $x + y + z = n - 4$ and $H(x, y, z)$ is obtained from $G[V_{3^+}]$ by adding x vertices of degree two adjacent to both u_2 and u_3, adding y vertices of degree two adjacent to both u_3 and u_4 and adding z vertices of degree two adjacent to both u_4 and u_2. Then we have $H(x, y, z) \cong X_1^{n-4}$. Now, we have

$$ABC(H(x,y,z)) = \sqrt{\frac{4+x}{3(3+x)}} + \sqrt{\frac{4+y}{3(3+y)}} + \sqrt{\frac{4+z}{3(3+z)}} + \sqrt{\frac{4+x+y}{(3+x)(3+y)}} + \sqrt{\frac{4+x+z}{(3+x)(3+z)}} + \sqrt{\frac{4+z+y}{(3+z)(3+y)}}.$$

By similar argument to the proof of Lemma 19, we have $ABC(H(x, y, z)) \leq ABC(H(0, 0, x + y + z)) = ABC(X_1^{n-4})$. Moreover, $ABC(H(x, y, z)) < ABC(X_1^{n-4})$ if $x + y > 0$. This assertion completes the proof. □

Theorem 1: Let G be an (n, m)-graph with $n \geq 5$ and $m = 2n - 2$. If $\delta(G) \geq 2$, then we have

$$ABC(G) \leq \max\{ABC(X_1^{n-4}), ABC(X_2^{n-5})\}.$$

Moreover, the equality holds if and only if either i) $G \cong X_1^{n-4}$ and $n \leq 34$, or (ii) $G \cong X_2^{n-5}$ and $n \geq 35$.

Proof: If $n \in \{5, 6, 7, 8, 9\}$, we can verify that $G \cong X_1^{n-4}$ by computer search. By Lemmas 4-20, we have $\mathcal{G} = \emptyset$. Therefore, if G is a graph with $n \geq 10$ vertices and $m = 2n-2$ edges, minimum degree at least two and the maximum ABC index, then $G \cong X_1^{n-4}$ or $G \cong X_2^{n-5}$. Then by Lemma 1, it follows that Theorem 1 holds. □

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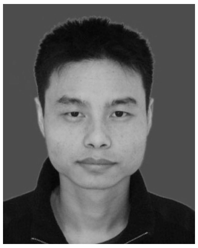

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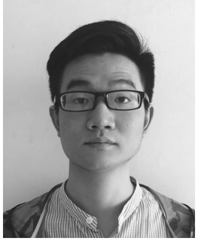

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