MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **85** (2021) 121-130

ISSN 0340 - 6253

On the Maximal General ABC Index of Graphs with Fixed Maximum Degree

Xuegong Tan[1], Muhuo Liu[2], Jianping Liu[3]

[1] *The College of Chinese Language and Culture, Jinan University, Guangzhou, 510610, China*
tanxuegong@hwy.jnu.edu.cn

[2] *Department of Mathematics, South China Agricultural University, Guangzhou, 510642, China*
liumuhuo@163.com (Corresponding author)

[3] *College of Mathematics and Computer Science, Fuzhou University, Fuzhou 350108, P.R. China*
ljping010@163.com

(Received June 10, 2020)

Abstract

As a generalization of the famous atom-bond connectivity index $ABC(G)$, the general atom-bound connectivity index of a graph G, $ABC_\alpha(G)$, is denoted by

$$ABC_\alpha(G) = \sum_{uv \in E(G)} \left(\frac{d_G(u) + d_G(v) - 2}{d_G(u) d_G(v)} \right)^\alpha \text{ for any } \alpha \in \mathbb{R} \setminus \{0\}.$$

The (general) atom-bound connectivity index has been shown to be a useful topological index and has received more and more attention recently. In this paper, we show that $ABC_\alpha(G + uv) > ABC_\alpha(G)$ holds for any two non-adjacent vertices u and v of a graph G with $d_G(u) + d_G(v) \geq 1$ for $0 < \alpha \leq \frac{1}{2}$. Moreover, by applying this new property, we determine the maximum value of ABC_α together with the corresponding extremal graphs in the class of graphs with n vertices and maximum degree Δ for $0 < \alpha \leq \frac{1}{2}$.

1 Introduction

Throughout this paper, we only consider undirected simple graphs, and $G = (V, E)$ is a simple graph. Let $d_G(u)$ and $N_G(x)$, respectively, be the degree and neighbor set of vertex u in G. Specially, $\Delta = \Delta(G)$ and $\delta = \delta(G)$, respectively, denotes the maximum and minimum degree of G. If $\Delta = \delta$, then G is called a **regular** graph. As in [3], if $\delta < \Delta$ and G contains exactly $|V(G)| - 1$ vertices of degree Δ and one vertex of degree δ, then G is called a (Δ, δ)**-quasi-regular** graph.

To study the strain energy of cycloalkanes and the stability of alkanes, E. Estrada et al. [4] put forward the notation of **atom-bond connectivity index**, $ABC(G)$ for a graph G, where

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

Later, to better understand the correlation properties of the atom-bond connectivity index for the heat of formation of alkanes, B. Furtula et al. [7] generalized the atom-bond connectivity index to the **general atom-bond connectivity index** $ABC_\alpha(G)$, where

$$ABC_\alpha(G) = \sum_{uv \in E(G)} \left(\frac{d_G(u) + d_G(v) - 2}{d_G(u)d_G(v)} \right)^\alpha \text{ for any } \alpha \in \mathbb{R} \setminus \{0\}. \tag{1}$$

It is easily checked that $ABC(G) = ABC_{\frac{1}{2}}(G)$.

Throughout this paper, denote by

$$\alpha_1 = \frac{\log\left(\frac{2\Delta-2}{2\Delta-3}\right)}{\log\left(\frac{\Delta^2}{4\Delta-4}\right)},\ \alpha_2 = \frac{\log\left(\frac{4\Delta-5}{4\Delta-6}\right)}{\log\left(\frac{\Delta^2}{4\Delta-4}\right)},\ \text{and } \alpha_3 = \frac{\log\left(\Delta - 1\right)}{\log\left(\frac{\Delta(2\Delta-3)}{2(\Delta-1)^2}\right)}.$$

Let $\mathcal{S}(n, \Delta)$ be the set of graphs with n vertices and maximum degree Δ. Recently, the research on extremal problem of (general) atom-bond connectivity index has received much attention [2, 3, 5, 6, 8, 9]. In this line, Chen et al. [2] showed the following useful property of ABC_α for connected graphs.

Theorem 1.1. [2] *Let G be a connected graph with two non-adjacent vertices u and v. If $\alpha \leq 1/2$ and $\alpha \neq 0$, then $ABC_\alpha(G + uv) > ABC_\alpha(G)$.*

In this paper, we will extent Theorem 1.1 to general graphs for $0 < \alpha \leq 1/2$.

Theorem 1.2. *Let G be a graph with two non-adjacent vertices u and v. If $0 < \alpha \leq 1/2$, then $ABC_\alpha(G + uv) \geq ABC_\alpha(G)$, where the equality holds if and only if u and v are two isolated vertices of G.*

Except for this, we shall consider the maximum general atom-bond connectivity index in the class of $\mathcal{S}(n, \Delta)$. If $\Delta = 1$, then $\mathcal{S}(n, \Delta)$ is the set of graphs with each component being either an edge or an isolated vertex. If $\Delta = 2$, then $\mathcal{S}(n, \Delta)$ is the set of graphs with each component being either a cycle or a path or an isolated vertex. Thus, we always suppose that $\Delta \geq 3$ in the following.

Theorem 1.3. [3] *Let G be a graph of $\mathcal{S}(n,\Delta)$, where $3 \le \Delta \le n-1$.*
(i) If Δn is even and $\alpha < \alpha_1$, then

$$ABC_\alpha(G) \le \frac{n\Delta}{2}\left(\frac{2\Delta-2}{\Delta^2}\right)^\alpha,$$

with equality if and only if G is regular.
(ii) If Δn is odd and $0 < \alpha \le \alpha_2$, then

$$ABC_\alpha(G) \le \frac{\Delta n - 2\Delta + 1}{2}\left(\frac{2\Delta-2}{\Delta^2}\right)^\alpha + (\Delta-1)\left(\frac{2\Delta-3}{\Delta(\Delta-1)}\right)^\alpha,$$

with equality if and only if G is $(\Delta,\Delta-1)$-quasi-regular.
(iii) If Δn is odd and $\alpha < 0$, then

$$ABC_\alpha(G) \le \max\left\{\frac{\Delta(n-1)-2d}{2}\left(\frac{2\Delta-2}{\Delta^2}\right)^\alpha + 2d\left(\frac{\Delta+2d-2}{2d\Delta}\right)^\alpha : 1 \le d \le \frac{\Delta-1}{2}\right\}.$$

(iv) If Δn is odd and $\alpha \le -\alpha_3$, then

$$ABC_\alpha(G) \le \frac{\Delta(n-1)-2}{2}\left(\frac{2\Delta-2}{\Delta^2}\right)^\alpha + 2^{1-\alpha},$$

with equality if and only if G is $(\Delta,2)$-quasi-regular.

A **chemical graph** is a connected graph with maximum degree $\Delta \le 4$. Let $\mathcal{C}(n,\Delta)$ be the class of connected chemical graphs with n vertices and maximum degree Δ. Except for Theorem 1.3 (which is not necessary connected), Das et al. [3] also determined the extremal maximum graphs in the class of $\mathcal{C}(n,\Delta)$, that is,

Theorem 1.4. [3] *Suppose that $3 \le \Delta \le 4$ and $\alpha \le \frac{1}{2}$ with $\alpha \ne 0$.*
(i) If Δn is even, then the graphs in $\mathcal{C}(n,\Delta)$ that maximize the ABC_α index are exactly the connected regular graphs.
(ii) If Δn is odd, then the graphs in $\mathcal{C}(n,\Delta)$ that maximize the ABC_α index are exactly the connected $(\Delta,\Delta-1)$-quasi-regular graphs.

Note that

$$\lim_{\Delta\to+\infty}\alpha_1 = \lim_{\Delta\to+\infty}\alpha_2 = 0, \text{ and } \lim_{\Delta\to+\infty}\alpha_3 = +\infty.$$

By comparing the results of Theorems 1.3 and 1.4 and since $ABC(G) = ABC_{\frac{1}{2}}(G)$, we will consider the similar problem for ABC_α in the case $0 < \alpha \le 1/2$, that is,

Theorem 1.5. *Let $G \in \mathcal{S}(n,\Delta)$, where $3 \le \Delta \le n-1$, and providing that $0 < \alpha \le 1/2$.*
(i) If Δn is even, then

$$ABC_\alpha(G) \le \frac{n\Delta}{2}\left(\frac{2\Delta-2}{\Delta^2}\right)^2,$$

where the equality holds if and only if G is regular.
(ii) If Δn is odd, then

$$ABC_\alpha(G) \le \frac{\Delta(n-2)+1}{2}\left(\frac{2\Delta-2}{\Delta^2}\right)^\alpha + (\Delta-1)\left(\frac{2\Delta-3}{\Delta(\Delta-1)}\right)^\alpha,$$

where the equality holds if and only if G is $(\Delta,\Delta-1)$-quasi-regular.

The extremal graphs of Theorem 1.5 must exist, as we have

Proposition 1.6. [1] *Suppose that $2 \le k \le n-1$.*

(i) If kn is even, then there is a connected k-regular graph with n vertices.

(ii) If kn is odd, then there is a connected $(k,k-1)$-quasi-regular graph with n vertices.

2 The proof of Theorem 1.2

This section is dedicated to the proof of Theorem 1.2. Hereafter, denote by

$$\Psi(x,y) = \left(\frac{x+y-1}{(x+1)y}\right)^\alpha - \left(\frac{x+y-2}{xy}\right)^\alpha.$$

Lemma 2.1. *Let x, y and α be three real numbers. If $x \ge 1$, $y > 0$ and $0 < \alpha < 1$, then*

$$\Psi(x,y) > \frac{-\alpha}{x(x+1)^\alpha}. \tag{2}$$

Proof. If $y = 2$, then $\Psi(x,y) = 0$, and so (2) holds. Next, we suppose that $y \ne 2$. To show (2), we define $\Phi(z) = z^\alpha$, let $z_1 = \frac{x+y-1}{(x+1)y}$ and $z_2 = \frac{x+y-2}{xy}$.

By the Lagrange Mean Value Theorem and since

$$z_1 - z_2 = \frac{x+y-1}{(x+1)y} - \frac{x+y-2}{xy} = \frac{2-y}{xy(x+1)},$$

we have

$$\Psi(x,y) = \Phi(z_1) - \Phi(z_2) = \alpha(z_1 - z_2)\xi^{\alpha-1} = \frac{\alpha(2-y)}{xy(x+1)}\xi^{\alpha-1}, \tag{3}$$

where $\xi \in (z_2, z_1)$ if $0 < y < 2$, and $\xi \in (z_1, z_2)$ if $y > 2$.

If $0 < y < 2$, then $\Phi(z_1) - \Phi(z_2) > 0$ by (3), and thus (3) implies that (2) holds.

If $y > 2$, then (3) implies that

$$\begin{aligned}\Phi(z_1) - \Phi(z_2) &> \frac{\alpha(2-y)}{xy(x+1)} \left(\frac{x+y-1}{(x+1)y}\right)^{\alpha-1} \\ &= \frac{\alpha(2-y)}{x(x+y-1)(x+1)^\alpha} \left(\frac{x+y-1}{y}\right)^{\alpha} \geq \frac{\alpha(2-y)}{xy(x+1)^\alpha} > \frac{-\alpha}{x(x+1)^\alpha},\end{aligned}$$

and thus (3) implies that (2) holds. ■

Lemma 2.2. *Let x and α be two real numbers. If $x \geq 3$ and $0 < \alpha \leq \frac{1}{2}$, then*

$$\frac{3}{2}\left(\frac{1}{2}\right)^\alpha > \left(\frac{x-1}{x}\right)^\alpha.$$

Proof. Since $\frac{4}{3} \leq \frac{2(x-1)}{x} < 2$ and $0 < \alpha \leq \frac{1}{2}$,

$$\left(\frac{2(x-1)}{x}\right)^\alpha < 2^\alpha \leq \sqrt{2} < \frac{3}{2}$$

and thus the result holds. ■

Proof of Theorem 1.2: Throughout this proof, we simplify write $d_G(x)$ and $N_G(x)$ as $d(x)$ and $N(x)$, respectively. Without loss of generality, we suppose that $d(u) \geq d(v)$.

Case 1. $d(v) = 0$.

If $d(u) = 0$, then $ABC_\alpha(G + uv) = ABC_\alpha(G)$ by (1).

If $d(u) = 1$, then suppose that $N(u) = w$, and thus $d(w) \geq 1$. By (1), we have

$$ABC_\alpha(G + uv) - ABC_\alpha(G) = 2\left(\frac{1}{2}\right)^\alpha - \left(\frac{d(w)-1}{d(w)}\right)^\alpha, \tag{4}$$

which implies that $ABC_\alpha(G + uv) > ABC_\alpha(G)$ for $1 \leq d(w) \leq 2$. Thus, we suppose that $d(w) \geq 3$ and then $ABC_\alpha(G + uv) > ABC_\alpha(G)$ follows from (4) and Lemma 2.2.

Next, we suppose that $d(u) \geq 2$. In this case, by (1) and Lemma 2.1, we have

$$\begin{aligned}ABC_\alpha(G + uv) - ABC_\alpha(G) &= \sum_{x \in N(u)} \Psi\big(d(u), d(x)\big) + \left(\frac{d(u)}{d(u)+1}\right)^\alpha \\ &> -\alpha\left(\frac{1}{d(u)+1}\right)^\alpha + \left(\frac{d(u)}{d(u)+1}\right)^\alpha.\end{aligned} \tag{5}$$

Since $d(u)^\alpha - \alpha \geq 2^\alpha - \alpha > 1 - \alpha > 0$, it follows from (5) that

$$ABC_\alpha(G + uv) - ABC_\alpha(G) > \frac{d(u)^\alpha - \alpha}{(d(u)+1)^\alpha} > 0,$$

as desired.

Case 2. $d(v) \geq 1$. By (1) and Lemma 2.1, we have

$$\begin{aligned}
&ABC_\alpha(G+uv) - ABC_\alpha(G) \\
=&\sum_{x\in N(u)} \Psi\big(d(u), d(x)\big) + \sum_{y\in N(v)} \Psi\big(d(v), d(y)\big) + \left(\frac{d(u)+d(v)}{\big(d(u)+1\big)\big(d(v)+1\big)}\right)^\alpha \\
>&\frac{-\alpha}{\big(d(u)+1\big)^\alpha} + \frac{-\alpha}{\big(d(v)+1\big)^\alpha} + \left(\frac{d(u)+d(v)}{\big(d(u)+1\big)\big(d(v)+1\big)}\right)^\alpha \\
\geq&\frac{-2\alpha}{\big(d(v)+1\big)^\alpha} + \frac{1}{\big(d(v)+1\big)^\alpha}\left(\frac{d(u)+d(v)}{d(u)+1}\right)^\alpha.
\end{aligned}$$

Since $0 < \alpha \leq \frac{1}{2}$ and $d(u) \geq d(v) \geq 1$, we have

$$\left(\frac{d(u)+d(v)}{d(u)+1}\right)^\alpha \geq 1 \geq 2\alpha.$$

Thus, $ABC_\alpha(G+uv) > ABC_\alpha(G)$, as desired. ■

3 The Proof of Theorem 1.5

Let $H(p)$ be a graph with $n-1$ vertices of degree Δ and one vertex of degree p, where $0 \leq p \leq \Delta$. From the definition, $H(\Delta)$ is a regular graph.

Lemma 3.1. *If $0 \leq p < q \leq \Delta$, $\Delta \geq 2$ and $0 < \alpha \leq \frac{1}{2}$, then*

$$ABC_\alpha\big(H(p)\big) < ABC_\alpha\big(H(q)\big).$$

Proof. We first suppose that $p = 0$. Since $0 < q \leq \Delta$, we have

$$\frac{\Delta+q-2}{q\Delta} \geq \frac{2\Delta-2}{\Delta^2} \text{ and thus } \left(\frac{\Delta+q-2}{q\Delta}\right)^\alpha \geq \left(\frac{2\Delta-2}{\Delta^2}\right)^\alpha.$$

From (1), it follows that

$$\begin{aligned}
&ABC_\alpha\big(H(q)\big) - ABC_\alpha\big(H(0)\big) \\
=&\frac{\Delta(n-1)-q}{2}\left(\frac{2\Delta-2}{\Delta^2}\right)^\alpha + q\left(\frac{\Delta+q-2}{q\Delta}\right)^\alpha - \frac{\Delta(n-1)}{2}\left(\frac{2\Delta-2}{\Delta^2}\right)^\alpha \\
\geq&\frac{\Delta(n-1)+q}{2}\left(\frac{2\Delta-2}{\Delta^2}\right)^\alpha - \frac{\Delta(n-1)}{2}\left(\frac{2\Delta-2}{\Delta^2}\right)^\alpha > 0,
\end{aligned}$$

as desired.

Next we suppose that $p \geq 1$. By (1), it suffices to show that

$$\begin{aligned}
\frac{\Delta(n-1)-q}{2}\left(\frac{2\Delta-2}{\Delta^2}\right)^\alpha + q\left(\frac{\Delta+q-2}{q\Delta}\right)^\alpha > &\frac{\Delta(n-1)-p}{2}\left(\frac{2\Delta-2}{\Delta^2}\right)^\alpha \\
&+ p\left(\frac{\Delta+p-2}{p\Delta}\right)^\alpha,
\end{aligned}$$

which is equivalent to

$$q\left(\frac{\Delta+q-2}{q\Delta}\right)^{\alpha}-p\left(\frac{\Delta+p-2}{p\Delta}\right)^{\alpha}>\frac{q-p}{2}\left(\frac{2\Delta-2}{\Delta^2}\right)^{\alpha}. \qquad (6)$$

Denote by $f(x)=x\left(\frac{\Delta+x-2}{x\Delta}\right)^{\alpha}$, where $x\geq 1$. By the Lagrange Mean Value Theorem, there exists θ with $p<\theta<q$ such that

$$(q-p)f'(\theta)=f(q)-f(p)=q\left(\frac{\Delta+q-2}{q\Delta}\right)^{\alpha}-p\left(\frac{\Delta+p-2}{p\Delta}\right)^{\alpha}$$

$$=(q-p)\left(\frac{\theta+(1-\alpha)(\Delta-2)}{\Delta+\theta-2}\right)\left(\frac{\Delta+\theta-2}{\theta\Delta}\right)^{\alpha}. \qquad (7)$$

Since $p<\theta<q\leq\Delta$ and $\Delta\geq 2$,

$$\frac{\Delta+\theta-2}{\theta\Delta}\geq\frac{\Delta+q-2}{q\Delta}\geq\frac{2\Delta-2}{\Delta^2}.$$

and thus $0<\alpha\leq\frac{1}{2}$ implies that

$$\left(\frac{\Delta+\theta-2}{\theta\Delta}\right)^{\alpha}\geq\left(\frac{2\Delta-2}{\Delta^2}\right)^{\alpha}. \qquad (8)$$

By Combining with (7) and (8), to show (6), it suffices to show that

$$\frac{\theta+(1-\alpha)(\Delta-2)}{\Delta+\theta-2}>\frac{1}{2}, \text{ that is } 2\big(\theta+(1-\alpha)(\Delta-2)\big)-\big(\Delta+\theta-2\big)>0. \qquad (9)$$

Since $1\leq p<\theta<q\leq\Delta$, $\Delta\geq 2$ and $0<\alpha\leq\frac{1}{2}$, we have $2\big(\theta+(1-\alpha)(\Delta-2)\big)-\big(\Delta+\theta-2\big)=\theta+(\Delta-2)(1-2\alpha)\geq\theta>0$, and so (9) holds. ■

Lemma 3.2. *Let G be a graph with two edges $\{uv,wz\}\subseteq E(G)$, where $d_G(v)>d_G(w)\geq d_G(z)$ and $d_G(u)=d_G(v)\geq 2$. If $0<\alpha<1$ and $\{uw,vz\}\nsubseteq E(G)$, then $ABC_\alpha(G_1)>ABC_\alpha(G)$, where $G_1=G+uw+vz-uv-wz$.*

Proof. For simplification, we rewrite $d_G(v)$, $d_G(w)$, and $d_G(z)$ as d, d_1 and d_2, respectively. By the hypothesis, we have $d>d_1\geq d_2$. To show that $ABC_\alpha(G_1)>ABC_\alpha(G)$, from (1) it suffices to show that

$$\left(\frac{d+d_1-2}{dd_1}\right)^{\alpha}+\left(\frac{d+d_2-2}{dd_2}\right)^{\alpha}>\left(\frac{2d-2}{d^2}\right)^{\alpha}+\left(\frac{d_1+d_2-2}{d_1d_2}\right)^{\alpha}. \qquad (10)$$

If $d_2=1$, since

$$\frac{d+d_1-2}{dd_1}\geq\frac{2d-2}{d^2},\ \frac{d-1}{d}>\frac{d_1-1}{d_1}, \text{ and } 0<\alpha<1,$$

it is easily checked that (10) already holds. Thus, we may suppose that $d_2 \geq 2$ and $d \geq 3$ in what follows. Now, to show (10), it suffices to show that

$$\int_{\frac{1}{d}\left(1-\frac{2}{d}\right)+\frac{1}{d}}^{\frac{1}{d_1}\left(1-\frac{2}{d}\right)+\frac{1}{d}} \alpha t^{\alpha-1} dt > \int_{\frac{1}{d}\left(1-\frac{2}{d_2}\right)+\frac{1}{d_2}}^{\frac{1}{d_1}\left(1-\frac{2}{d_2}\right)+\frac{1}{d_2}} \alpha t^{\alpha-1} dt,$$

which is equivalent to

$$\int_{\frac{1}{d}\left(1-\frac{2}{d}\right)}^{\frac{1}{d_1}\left(1-\frac{2}{d}\right)} \alpha \left(t+\frac{1}{d}\right)^{\alpha-1} dt > \int_{\frac{1}{d}\left(1-\frac{2}{d_2}\right)}^{\frac{1}{d_1}\left(1-\frac{2}{d_2}\right)} \alpha \left(t+\frac{1}{d_2}\right)^{\alpha-1} dt. \tag{11}$$

By Mean Value Theorem of Integrals, $\frac{1}{d_1} > \frac{1}{d}$ and $0 < \alpha < 1$, (11) is equivalent to

$$\left(1-\frac{2}{d}\right)\left(\theta_1+\frac{1}{d}\right)^{\alpha-1} > \left(1-\frac{2}{d_2}\right)\left(\theta_2+\frac{1}{d_2}\right)^{\alpha-1}, \tag{12}$$

where $\frac{1}{d}\left(1-\frac{2}{d}\right) \leq \theta_1 \leq \frac{1}{d_1}\left(1-\frac{2}{d}\right)$ and $\frac{1}{d}\left(1-\frac{2}{d_2}\right) \leq \theta_2 \leq \frac{1}{d_1}\left(1-\frac{2}{d_2}\right)$.

Once again, since $0 < \alpha < 1$ and $1-\frac{2}{d_2} < 1-\frac{2}{d}$, to prove (12), it suffices to show that

$$0 < \theta_1 + \frac{1}{d} \leq \theta_2 + \frac{1}{d_2}. \tag{13}$$

Taking $\frac{1}{d}\left(1-\frac{2}{d}\right) \leq \theta_1 \leq \frac{1}{d_1}\left(1-\frac{2}{d}\right)$, $\theta_2 \geq \frac{1}{d}\left(1-\frac{2}{d_2}\right)$ and $d \geq 2$ into consideration, it follows that

$$0 < \frac{1}{d}\left(2-\frac{2}{d}\right) \leq \theta_1 + \frac{1}{d} \leq \frac{1}{d_1}\left(1-\frac{2}{d}\right) + \frac{1}{d} \leq \frac{1}{d}\left(1-\frac{2}{d_2}\right) + \frac{1}{d_2} \leq \theta_2 + \frac{1}{d_2},$$

and thus (13) holds. ■

Proof of Theorem 1.5: Let $G \in \mathcal{S}(n, \Delta)$ be a graph with maximal $ABC_\alpha(G)$. Denote by $V_1 = \{v \in V(G) : d_G(v) < \Delta\}$ and $V_2 = \{u \in V(G) : d_G(u) = \Delta\}$. Suppose that $|V_1| = k$. By Theorem 1.2, we can conclude that $G[V_1] \cong K_k$. Otherwise, if $G[V_1] \ncong K_k$, then we can add some edges to $G[V_1]$ so that the resultant graph has larger ABC_α index than G and also belongs to $\mathcal{S}(n, \Delta)$, contrary with the choice of G and Theorem 1.2.

By the definition of V_1, we have $0 \leq k = |V_1| \leq \Delta$. Now, we prove $|V_1| \leq 1$.

Claim 1. If $|V_1| = k \geq 1$, then $N_G(x) \cap V_2 \neq \emptyset$ for some vertex x of V_1.

Proof of Claim 1. By contradiction, we assume that $G[V_1] = K_k$ is a component of G. If $k \geq 2$, then there exists one edge of $G[V_1]$. Note that $G[V_2]$ contains at least one edge. Thus, by the operation as defined in Lemma 3.2, it leads to a contradiction. Therefore, $k = 1$. In this case, $G[V_1]$ is an isolated vertex. By Lemma 3.1, $ABC_\alpha(G)$ is not maximum, a contradiction. This completes the proof of Claim 1. ■

In what follows, by Claim 1, if $|V_1| = k \geq 1$, then we always suppose that

$$x \text{ is a vertex of } V_1 \text{ such that } N_G(x) \cap V_2 \neq \emptyset \text{ and } u \in N_G(x) \cap V_2. \tag{14}$$

Claim 2. If $|V_1| = k \geq 2$, then u is adjacent to every vertex of V_1.

Proof of Claim 2. Let $N_G(x) \cap V_2 = S$ and $V_2 - S = T$. By (14), we have $|S| + |V_1| - 1 = d_G(x) \leq \Delta - 1 < d_G(u)$, and $S \neq \emptyset$, which implies that $T \neq \emptyset$.

For any vertex u of S, since $d_G(u) = \Delta > d_G(x) = |S|+|V_1|-1$, we have $N_G(u) \cap T \neq \emptyset$, and thus we may suppose that $uv \in E(G)$, where $v \in T$. If there exists some vertex y of V_1 such that $uy \notin E(G)$, then $xy \in E(G)$, as $G[V_1] = K_k$. Since $u \in S$ and $v \in T$, we can define $G_1 = G + uy + vx - uv - xy$. In this case, $G_1 \in \mathcal{S}(n, \Delta)$. However, Lemma 3.2 implies that $ABC_\alpha(G_1) > ABC_\alpha(G)$, a contradiction. Thus, u is adjacent to every vertex of V_1, and so Claim 2 holds. ■

By Claim 2, we can conclude that

$$N_G(x) \setminus \{y\} = N_G(y) \setminus \{x\} \text{ holds for any two vertices } \{x, y\} \subseteq V_1. \tag{15}$$

Claim 3. $|V_1| = k \leq 1$.

Proof of Claim 3. By contradiction, we assume that $|V_1| = k \geq 2$. Recall that $S = N_G(x) \cap V_2$ and $T = V_2 \backslash S$, where x is defined as in (14). As in the proof of Claim 2, if $|V_1| \geq 2$, then $S \neq \emptyset \neq T$.

If $E\big(G[T]\big) \neq \emptyset$, then we choose $u_0v_0 \in E\big(G[T]\big)$ and $xy \in E\big(G[V_1]\big)$ (as $k \geq 2$, such edge xy must exist). By (15), $N_G(y) \cap T = \emptyset = N_G(x) \cap T$. Let $G_2 = G + u_0x + v_0y - u_0v_0 - xy$. Then, $G_2 \in \mathcal{S}(n, \Delta)$ and $ABC_\alpha(G_2) > ABC_\alpha(G)$ by Lemma 3.2. This contradiction shows that $G[T]$ is an independent set of G. We choose $w \in T$. Then, $N_G(w) \subseteq S$ by (15). This implies that $\Delta = d_G(w) \leq |S| < |S| + |V_1| - 1 = d_G(x) < \Delta$, a contradiction. Thus, Claim 3 holds. ■

In what follows, we divide the proof into two cases according to the parity of $n\Delta$.

Case 1. $n\Delta$ is even. In this case, to complete the proof of Theorem 1.5 (i), it suffices to show that $|V_1| = k = 0$. By contradiction and Claim 3, we assume that $|V_1| = 1$, and suppose that $d_G(z) = \delta < \Delta$. Then, $G = H(\delta)$ and thus $ABC_\alpha(G) = ABC_\alpha\big(H(\delta)\big) < ABC_\alpha\big(H(\Delta)\big)$ by Lemma 3.1 and Proposition 1.6 (i), a contradiction.

Case 2. $n\Delta$ **is odd.** Since $n\Delta$ is odd, by the Handshaking Lemma, G is not a regular graph, that is $\delta < \Delta$. By Claim 3, G is a (Δ, δ)-quasi-regular graph. To complete the proof of Theorem 1.5 (ii), it suffices to show that $\delta = \Delta - 1$. By contradiction, if $\delta \leq \Delta - 2$, then $ABC_\alpha(G) = ABC_\alpha\big(H(\delta)\big) < ABC_\alpha\big(H(\Delta - 1)\big)$ by Lemma 3.1 and Proposition 1.6 (ii), a contradiction. ■

Acknowledgment: The third author is supported by the Natural Science Foundation of Fujian Province (2019J01643).

References

[1] W. Carballosa, J. M. Rodríguez, J. M. Sigarreta, Inequalities and several extremal problems on the variable sum exdeg index, submitted.

[2] X. Chen, G. Hao, Extremal graphs with respect to generalized *ABC* index, *Discr. Appl. Math.* **243** (2018) 115–124.

[3] K. C. Das, J. M. Rodríguez, J. M. Sigarreta, On the maximal general *ABC* index of graphs with given maximum degree, *Appl. Math. Comput.*, to appear.

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

[5] I. Gutman, B. Furtula, Trees with smallest atom-bond connectivity index, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 131–136.

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

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

[8] R. Xing, B. Zhou, F. Dong, On atom–bond connectivity index of connected graphs, *Discr. Appl. Math.* **159** (2011) 1617–1630.

[9] X. M. Zhang, Y. Yang, H. Wang, X. D. Zhang, Maximum atom–bond connectivity index with given graph parameters, *Discr. Appl. Math.* **215** (2016) 208–217.