Filomat 38:19 (2024), 6639–6650
https://doi.org/10.2298/FIL2419639B

Published by Faculty of Sciences and Mathematics,
University of Niš, Serbia
Available at: http://www.pmf.ni.ac.rs/filomat

On minimum generalized ABC index of graphs

Lkhagva Buyantogtokh[a], Batmend Horoldagva[a,*], Ivan Gutman[b]

[a] *Department of Mathematics, Mongolian National University of Education, Baga toiruu-14, Ulaanbaatar, Mongolia*
[b] *Faculty of Science, University of Kragujevac, P.O.Box 60, 34000 Kragujevac, Serbia*

Abstract. The generalized ABC index of a graph G, denoted by ABC_α, is defined as the sum of the terms $[(d(v)+d(u)-2)/d(v)d(u)]^\alpha$ over all pairs of adjacent vertices, where $d(u)$ is the degree of the vertex u and α is a real number. In this paper, we prove that for $\alpha \le -1$, the balanced double broom is the unique tree that minimizes ABC_α among trees of order n with diameter d, and trees of order n with k pendent vertices.

1. Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$, where $|V(G)| = n$ and $|E(G)| = m$. Denote by $d(v)$, the degree of the vertex v in G. The maximum degree of G is denoted by Δ. A pendent vertex is a vertex of degree one. For $v \in V(G)$, $N(v)$ denotes the set of neighbors of v. A tree of order n with maximum degree two is called a path and is denoted by P_n. A tree of order n with maximum degree $n-1$ is called a star and is denoted by S_n. Denote by C_g a cycle of length g. For a subset E of $E(G)$, we denote by $G-E$ the subgraph of G obtained from G by deleting the edges in E. Similarly, we denote by $G+E$ the supergraph of G obtained from G by adding the edges in E. If $E=\{e\}$, we write $G-e$ and $G+e$.

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

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

This degree-based graph invariant was introduced at the end of the 1990s by Estrada et al. [12]. Its chemical and mathematical properties are being intensively studied ever since. For a recent review on the mathematical propertires of the ABC index see [1]; details of its chemical applications are found in [11, 14].

A long time puzzling problem was the characterization of graphs with minimum ABC-value (which must be trees). Dozens of papers on this matter were published, containing partial results and (false)

2020 *Mathematics Subject Classification*. Primary 05C35, 05C90, 05C92; Secondary 05C05, 05C07, 05C09.
Keywords. atom-bond connectivity index; ABC index; augmented Zagreb index; balanced double broom.
Received: 12 October 2023; Accepted: 08 March 2024
Communicated by Dragan S. Djordjević
Research supported by the Mongolian Foundation for Science and Technology (Grant No. SHUTBIKHKHZG-2022/162).
* Corresponding author: Batmend Horoldagva
Email addresses: buyantogtokh.l@msue.edu.mn (Lkhagva Buyantogtokh), horoldagva@msue.edu.mn (Batmend Horoldagva), gutman@kg.ac.rs (Ivan Gutman)

conjectures. Finally, the problem was completely solved in 2023 [9, 10], revealing that the structure of the minimum ABC trees is rather perplexed.

Of the numerous other studies of ABC index, we mention the following. Shao et al. [21] characterized the graphs with n vertices, without pendent vertices, and m edges for $m = 2n - 4$ and $m = 2n - 3$, having maximum ABC index. Zhang et al. [24] described the structural properties of graphs having minimum ABC index among connected graphs with a given degree sequence. Moreover, they characterized the extremal graphs having minimum ABC among unicyclic and bicyclic graphs with a given degree sequence. Lower and upper bounds on ABC in terms of Randić index, first Zagreb index, second Zagreb index, and modified second Zagreb index were reported in [6]. Chen and Das [4] proved that among n-vertex graphs with given chromatic number, the Turán graph is the unique graph having the maximum ABC index. Shao et al. [22] reported a sharp upper bound for bipartite graphs of order $n \geq 6$, size $2n - 3$, and with no pendent vertex, and characterized all extreme bipartite graphs. Wu and Zhang [23] determined the minimum ABC index and its structural properties for chemical trees with n vertices and k pendent vertices for $n \geq 3k - 2$.

In order to obtain better correlation abilities of ABC index for the heat of formation of alkanes, Furtula et al. [13] proposed a generalization of this index as:

$$ABC_\alpha(G) = \sum_{vu \in E(G)} \left(\frac{d(u) + d(v) - 2}{d(u)\,d(v)} \right)^\alpha ,$$

where α is some non-zero real number. They established that $\alpha = -3$ yields the best correlation results, and named the respective index "augmented Zagreb index", AZI,

$$AZI(G) = \sum_{vu \in E(G)} \left(\frac{d(u)\,d(v)}{d(u) + d(v) - 2} \right)^3 .$$

Chen and Hao [5] characterized the graphs with maximal ABC_α-value for $\alpha < 0$ among connected graphs with given order and vertex connectivity, edge connectivity, or matching number. Das et al. [7] obtained some optimization results on ABC_α for connected graphs. Prakasha et al. [20] calculated the atom-bond connectivity index of some derived graphs, such as double graphs, subdivision graphs and complements of some standard graphs. A generalized version of ABC_α was studied in [3].

Evidently, ABC_α is the generalization of the augmented Zagreb index $AZI = ABC_{-3}$. Furtula et al. [13] proved that S_n is the unique extremal tree of order n with minimal AZI. Lin et al. [18] conjectured that the balanced double star is the unique tree of order n with maximum AZI for $n \geq 19$. Eventually, Lin et al. [19] proved this conjecture. Further results related to AZI can be found in the review [2], the papers, [8, 15–17], and the references cited therein.

In this paper, we prove that for $\alpha \leq -1$, the balanced double broom is the unique tree minimizing ABC_α among trees of order n and diameter d, as well as trees of order n with k pendent vertices.

2. Preliminaries

Let x_1, x_2 and α be positive real numbers such that $x_1, x_2, \alpha \geq 1$ and $x_1 + x_2 \geq 3$. Consider the function $f_\alpha(x_1, x_2) = [x_1\, x_2/(x_1 + x_2 - 2]^\alpha$. For $\alpha = 3$, some properties of this function were studied in [17–19]. In this section, we prove that analogous results hold for $f_\alpha(x_1, x_2)$ when $\alpha \geq 1$, and state some previously known results needed in the subsequent sections.

Lemma 2.1. *Let* $\alpha \geq 1$.
(i) *The function* $f_\alpha(x_1, 1)$ *strictly decreases for* $x_1 \geq 2$ *and* $f_\alpha(x_1, 2) = 2^\alpha$.
(ii) *For given* $x_2 \geq 3$, *the function* $f_\alpha(x_1, x_2)$ *strictly increases for* $x_1 \geq 2$.

Proof. (i) From the definition of $f_\alpha(x_1, x_2)$, we have

$$f_\alpha(x_1, 1) = \left(\frac{x_1}{x_1 - 1} \right)^\alpha = \left(1 + \frac{1}{x_1 - 1} \right)^\alpha$$

and

$$f_\alpha(x_1,2)=\left(\frac{2x_1}{2+x_1-2}\right)^\alpha=2^\alpha.$$

From the first equation, one can easily see that $f_\alpha(x_1,1)$ strictly decreases with $x_1\geq 2$.
(ii) Also, we have

$$f_\alpha(x_1,x_2)=\left(\frac{x_1x_2}{x_1+x_2-2}\right)^\alpha=\left(x_2-\frac{x_2^2-2x_2}{x_1+x_2-2}\right)^\alpha.$$

Since $x_2\geq 3$, we have $x_2^2-2x_2>0$ and it follows that $f_\alpha(x_1,x_2)$ strictly increases with $x_1\geq 2$. □

The following result immediately follows from the above lemma.

Lemma 2.2. *If $\alpha>0$, $x_1,x_2,x_3\geq 3$ and $x_4\geq 2$, then*

$$\begin{aligned}1 &< f_\alpha(x_3,1)\leq f_\alpha(3,1)=(3/2)^\alpha<f_\alpha(2,1)=f_\alpha(2,x_4)=2^\alpha\\ &< (9/4)^\alpha=f_\alpha(3,3)\leq f_\alpha(x_1,x_2),\end{aligned}$$

with equalities if and only if $x_3=3$ and $x_1=x_2=3$, respectively.

Lemma 2.3. [5] *Let G be a connected graph with non-adjacent vertices u and v. If $\alpha<0$, then $ABC_\alpha(G+uv)>ABC_\alpha(G)$.*

Let $x=(x_1,x_2,\ldots,x_n)$ and $y=(y_1,y_2,\ldots,y_n)$ be two sequences of real numbers. If the sequences x and y satisfy the following three conditions
(i) $x_1\geq x_2\geq\cdots\geq x_n$ and $y_1\geq y_2\geq\cdots\geq y_n$,
(ii) $x_1+x_2+\cdots+x_k\geq y_1+y_2+\cdots+y_k$, for all $1\leq k\leq n-1$,
(iii) $x_1+x_2+\cdots+x_n=y_1+y_2+\cdots+y_n$,
then one says that the sequence x majorizes the sequence y, which is denoted by $x\succ y$ or $y\prec x$.

Lemma 2.4. (Karamata's inequality) *Let $x=(x_1,x_2,\ldots,x_n)$ and $y=(y_1,y_2,\ldots,y_n)$ be sequences of real numbers on the interval (t_1,t_2). If $x\succ y$, and $f:(t_1,t_2)\to\mathbb{R}$ is a strictly convex function, then*

$$f(x_1)+f(x_2)+\cdots+f(x_n)\geq f(y_1)+f(y_2)+\cdots+f(y_n)$$

with equality if and only if $x_i=y_i$ for all i , $1\leq i\leq n$.

Lemma 2.5. (Power mean inequality) *Let $\beta\geq 1$ be a real number and $x_1,x_2,\ldots,x_r$ be non-negative real numbers. Then*

$$\frac{x_1^\beta+x_2^\beta+\cdots+x_r^\beta}{r}\geq\left(\frac{x_1+x_2+\cdots+x_r}{r}\right)^\beta,$$

with equality if and only if $x_1=x_2=\cdots=x_n$ or $\beta=1$.

Lemma 2.6. *Let c and $t_1\geq t_2>1$ be positive integers such that $t_1+t_2=c$. If $\beta>1$, then*

$$\frac{t_1^\beta}{(t_1-1)^{\beta-1}}+\frac{t_2^\beta}{(t_2-1)^{\beta-1}}\geq\frac{\lceil c/2\rceil^\beta}{(\lceil c/2\rceil-1)^{\beta-1}}+\frac{\lfloor c/2\rfloor^\beta}{(\lfloor c/2\rfloor-1)^{\beta-1}}$$

with equality if and only if $t_1=\lceil c/2\rceil$ and $t_2=\lfloor c/2\rfloor$.

Proof. Consider a function $f(t)=t^\beta/(t-1)^{\beta-1}$ for $t\geq 2$. Then we have

$$f'(t)=\frac{t^{\beta-1}(t-\beta)}{(t-1)^\beta}\quad\text{and}\quad f''(t)=\frac{\beta(\beta-1)t^{\beta-2}}{(t-1)^{\beta+1}}>0,$$

since $\beta>1$ and $t>1$. It follows that $f(t)$ is strictly convex on $(1,\infty)$. Also, one can easily see that (t_1,t_2) majorizes $(\lceil c/2\rceil,\lfloor c/2\rfloor)$, i. e.,

$$(t_1,t_2)\succ(\lceil c/2\rceil,\lfloor c/2\rfloor),$$

since $t_1\geq t_2$ are integers such that $t_1+t_2=c$. Hence by Karamata's inequality we get the required result. □

3. Graphs of order n with diameter d

A double broom $DB_{a,b,d}$ is a tree obtained from P_{d-1} by attaching $a-1$ and $b-1$ pendent edges, respectively, to its end vertices. If $|a-b| \le 1$ then the double broom is said to be balanced. If $d=3$, then a double broom $DB_{a,b,3}$ is called a double star and is denoted by $DS_{a,b}$. Denote by $\mathcal{T}_{n,d}$ the set of trees of order n with diameter d. Then it is easy to check that $DB_{a,b,d} \in \mathcal{T}_{n,d}$ when $a+b=n-d+3$, and any tree in $\mathcal{T}_{n,3}$ is a double star.

Theorem 3.1. *Let T be a tree in $\mathcal{T}_{n,3}$ and $\alpha \le -1$. Then*

$$ABC_\alpha(T) \ge \frac{2}{2^\alpha} + (n-3)\left(\frac{n-3}{n-2}\right)^\alpha$$

with equality if and only if T is isomorphic to the double star $DS_{n-2,2}$.

Proof. Since $T \in \mathcal{T}_{n,3}$, there exist positive integers $a \ge b \ge 2$, such that $a+b=n$ and $T \cong DS_{a,b}$. For convenience, we denote $\beta = -\alpha$. Then $\beta \ge 1$ and from the definition of ABC_α, we have

$$ABC_\alpha(DS_{a,b}) = \frac{a^\beta}{(a-1)^{\beta-1}} + \frac{b^\beta}{(b-1)^{\beta-1}} + \left(\frac{ab}{n-2}\right)^\beta,$$

because $a+b=n$. Therefore, it suffices to prove that

$$\frac{a^\beta}{(a-1)^{\beta-1}} + \frac{b^\beta}{(b-1)^{\beta-1}} + \left(\frac{ab}{n-2}\right)^\beta \ge 2^{\beta+1} + (n-3)\left(\frac{n-2}{n-3}\right)^\beta. \tag{1}$$

If $\beta = 1$, then $ab \ge 2(n-2)$ since $b \ge 2$ and $a+b=n$. Hence, we easily get the required result from (1).

Let now $\beta > 1$. If $b=2$. then one can easily see that the equality in (1) holds. Thus, we assume that $b \ge 3$ and prove that the strict inequality in (1) holds. From $a+b=n$ and $a \ge b \ge 3$, we have $n-2 > a \ge b \ge 3$ and it follows that

$$(a-1)\left(\frac{a}{a-1}\right)^\beta + (b-2)\left(\frac{b}{b-1}\right)^\beta > (n-3)\left(\frac{n-2}{n-3}\right)^\beta \tag{2}$$

by Lemma 2.1 and $a+b=n$. Since $b \ge 3$, we have $n \ge 6$.

Let $n \ge 8$. If $b=3$, then $ab = 3(n-3)$ and we have

$$\frac{b}{b-1} + \frac{ab}{n-2} = \frac{3}{2} + \frac{3(n-3)}{n-2} = \frac{9}{2} - \frac{3}{n-2} \ge \frac{9}{2} - \frac{3}{6} = 4.$$

If $b \ge 4$, then $ab \ge 4(n-4)$ and we get

$$\frac{b}{b-1} + \frac{ab}{n-2} \ge \frac{n/2}{n/2-1} + \frac{4(n-4)}{n-2} = 5 - \frac{6}{n-2} \ge 5 - \frac{6}{6} = 4.$$

since $b \le n/2$ and $ab \ge 4(n-4)$. Hence, by Lemma 2.5,

$$\left(\frac{b}{b-1}\right)^\beta + \left(\frac{ab}{n-2}\right)^\beta \ge 2\left[\frac{1}{2}\left(\frac{b}{b-1} + \frac{ab}{n-2}\right)\right]^\beta \ge 2^{\beta+1}, \tag{3}$$

since $\beta > 1$. Bearing in mind the inequalities (2) and (3), we arrive at the strict inequality in (1).

Consider now the cases $n=6$ or $n=7$. Then $a=b=3$ or $b=3$, $a=4$. Therefore, we need to prove that

$$4\left(\frac{3}{2}\right)^\beta + \left(\frac{9}{4}\right)^\beta \ge 2^{\beta+1} + 3\left(\frac{4}{3}\right)^\beta$$

and

$$2\left(\frac{3}{2}\right)^{\beta}+3\left(\frac{4}{3}\right)^{\beta}+\left(\frac{12}{5}\right)^{\beta}\geq 2^{\beta+1}+4\left(\frac{5}{4}\right)^{\beta}.$$

By direct numerical calculations, we check that the above inequalities hold for all $\beta \geq 1$. This completes the proof. □

If $d \geq 4$, then by using Lemma 2.1, we can directly calculate that

$$ABC_{\alpha}(DB_{a,b,d})=\frac{d-2}{2^{\alpha}}+\frac{(a-1)^{\alpha+1}}{a^{\alpha}}+\frac{(b-1)^{\alpha+1}}{b^{\alpha}}. \tag{4}$$

The above equation and $a+b=n-d+3$ imply the following lemma.

Lemma 3.2. *Let n and d be positive integers such that $n > d \geq 4$. If T is a double broom in $\mathcal{T}_{n,d}$, then*

$$ABC_{-1}(T)=n+d-1.$$

Theorem 3.3. *Let n and d be positive integers such that $n > d \geq 4$ and T be a tree in $\mathcal{T}_{n,d}$. If $\alpha \leq -1$, then*

$$ABC_{\alpha}(T)\geq\frac{d-2}{2^{\alpha}}+\frac{\lceil (n-d+1)/2\rceil^{\alpha+1}}{\lceil (n-d+3)/2\rceil^{\alpha}}+\frac{\lfloor (n-d+1)/2\rfloor^{\alpha+1}}{\lfloor (n-d+3)/2\rfloor^{\alpha}} \tag{5}$$

with equality if and only if T is isomorphic to a double broom in $\mathcal{T}_{n,d}$ when $\alpha=-1$, and T is isomorphic to the balanced double broom in $\mathcal{T}_{n,d}$ when $\alpha < -1$.

Proof. For convenience, denote $\beta=-\alpha$. Let $v_1v_2\cdots v_{d+1}$ be a diameter of T and u be a maximum degree vertex in T. Also let $N(u)=\{w_1,w_2,\ldots,w_{\Delta}\}$, $d(w_1)\geq 2$ and Δ_1 be the maximum degree in $V(T)\setminus\{u\}$. Clearly $\Delta_1 \geq 2$. For all i such that $2 \leq i \leq d$, we have $d(v_i) \geq 2$ and by Lemma 2.2 it follows that

$$f_{\beta}(d(v_i),d(v_{i+1}))\geq 2^{\beta}\quad\text{for all}\quad 2\leq i\leq d-1.$$

In addition, by Lemma 2.1,

$$f_{\beta}(d(u),d(w_i))\geq\left(\frac{\Delta}{\Delta-1}\right)^{\beta}\quad\text{for all}\ \ 2\leq i\leq\Delta.$$

For any edge xy in $E(T)$, different from $v_2v_3, v_3v_4, \ldots, v_{d-1}v_d$ and $uw_2, uw_3, \ldots, uw_{\Delta}$, we have

$$f_{\beta}(d(x),d(y))\geq\left(\frac{\Delta_1}{\Delta_1-1}\right)^{\beta},$$

by the definition of Δ_1 and Lemma 2.1. On the other hand, one can easily see that $\Delta_1 \leq n-d-\Delta+3$. Denote $M=\{v_2v_3, v_3v_4, \ldots, v_{d-1}v_d\}$ and $N=\{uw_2, uw_3, \ldots, uw_{\Delta}\}$. Then, from the above mentioned inequalities we get

$$
\begin{aligned}
ABC_\alpha(T) &\geq 2^\beta |M| + \Big(|N| - |M \cap N|\Big)\left(\frac{\Delta}{\Delta-1}\right)^\beta \\
&+ \Big(n-1-|M \cup N|\Big)\left(\frac{\Delta_1}{\Delta_1-1}\right)^\beta \qquad (6) \\
&\geq 2^\beta (d-2) + (\Delta-1)\left(\frac{\Delta}{\Delta-1}\right)^\beta - |M \cap N|\left(\frac{\Delta_1}{\Delta_1-1}\right)^\beta \\
&+ \Big(n-1-|M \cup N|\Big)\left(\frac{\Delta_1}{\Delta_1-1}\right)^\beta \\
&= 2^\beta (d-2) + (\Delta-1)\left(\frac{\Delta}{\Delta-1}\right)^\beta + (n-d-\Delta+2)\left(\frac{\Delta_1}{\Delta_1-1}\right)^\beta \\
&\geq 2^\beta (d-2) + (\Delta-1)\left(\frac{\Delta}{\Delta-1}\right)^\beta \\
&+ (n-d-\Delta+2)\left(\frac{n-d-\Delta+3}{n-d-\Delta+2}\right)^\beta \qquad (7)
\end{aligned}
$$

by $|E(T)| = n-1$, $|M| = d-2$, $|N| = \Delta - 1$, $\Delta_1 \leq \Delta$, $\Delta_1 \leq n-d-\Delta+3$.

Now we distinguish the following two cases.

Case 1. Let $\beta = 1$. Then from (7), we get

$$ABC_{-1}(T) \geq 2(d-2) + \Delta + (n-d-\Delta+3) = n+d-1\,,$$

which is our required result. If the equality in (5) holds, then the equality in (7) holds, and it follows that $\Delta_1 = n-d-\Delta+3$. Also the equality in (6) holds. Hence, all edges in $E(T) \setminus M$ are pendent and are adjacent to u or v, where v is the vertex such that $d(v) = \Delta_1$. Hence, one can easily see that T is isomorphic to a double broom in $\mathcal{T}_{n,d}$. Conversely, if T is isomorphic to a double broom in $\mathcal{T}_{n,d}$ then

$$ABC_{-1}(T) = n+d-1,$$

by Lemma 3.2.

Case 2. Let $\beta > 1$. Then from (7) and Lemma 2.6, we get

$$
\begin{aligned}
ABC_\alpha(T) &\geq (d-2)2^\beta + \frac{\Delta^\beta}{(\Delta-1)^{\beta-1}} + \frac{(n-d-\Delta+3)^\beta}{(n-d-\Delta+2)^{\beta-1}} \\
&\geq (d-2)2^\beta + \frac{\lceil (n-d+3)/2 \rceil^\beta}{\lceil (n-d+1)/2 \rceil^{\beta-1}} + \frac{\lfloor (n-d+3)/2 \rfloor^\beta}{\lfloor (n-d+1)/2 \rfloor^{\beta-1}} \qquad (8) \\
&= \frac{d-2}{2^\alpha} + \frac{\lceil (n-d+1)/2 \rceil^{\alpha+1}}{\lceil (n-d+3)/2 \rceil^{\alpha}} + \frac{\lfloor (n-d+1)/2 \rfloor^{\alpha+1}}{\lfloor (n-d+3)/2 \rfloor^{\alpha}}\,.
\end{aligned}
$$

If the equality in (5) holds, then also the equalities in (6) and (7) must hold. Hence, T is isomorphic to a double broom by Case 1. Also, the equality in (8) holds, and it follows that

$$\Delta = \lceil (n-d+3)/2 \rceil \quad \text{and} \quad \Delta_1 = \lfloor (n-d+3)/2 \rfloor\,.$$

Therefore, T is isomorphic to the balanced double broom in $\mathcal{T}_{n,d}$. □

Corollary 3.4. [15] *Let T be a tree of order n with diameter $d \geq 4$. Then*

$$AZI(T) \geq 8(d-2) + \frac{\lceil (n-d+3)/2 \rceil^3}{\lceil (n-d+1)/2 \rceil^2} + \frac{\lfloor (n-d+3)/2 \rfloor^3}{\lfloor (n-d+1)/2 \rfloor^2}$$

with equality if and only if T is isomorphic to the balanced double broom in $\mathcal{T}_{n,d}$.

Theorem 3.5. *Let T be a tree of order n. If $\alpha \leq -1$ then*

$$ABC_\alpha(T) \geq (n-1)\left(\frac{n-2}{n-1}\right)^\alpha$$

with equality if and only if T is isomorphic to the star S_n.

Proof. Let $\beta = -\alpha$ and d be the diameter of T. From Lemma 2.1, we have

$$\left(\frac{n-1}{n-2}\right)^\beta < \left(\frac{n-2}{n-3}\right)^\beta < \left(\frac{\lceil (n-d+3)/2 \rceil}{\lceil (n-d+1)/2 \rceil}\right)^\beta \leq \left(\frac{\lfloor (n-d+3)/2 \rfloor}{\lfloor (n-d+1)/2 \rfloor}\right)^\beta$$

since $n-1 > n-2 > \lceil (n-d+3)/2 \rceil \geq \lfloor (n-d+3)/2 \rfloor$. Hence, we get

$$(d-2)2^\beta + \frac{\lceil (n-d+3)/2 \rceil^\beta}{\lceil (n-d+1)/2 \rceil^{\beta-1}} + \frac{\lfloor (n-d+3)/2 \rfloor^\beta}{\lfloor (n-d+1)/2 \rfloor^{\beta-1}}$$

$$> 2 \cdot 2^\beta + (n-3)\left(\frac{n-2}{n-3}\right)^\beta > (n-1)\left(\frac{n-1}{n-2}\right)^\beta$$

since $2 > \frac{n-2}{n-3} > \frac{n-1}{n-2}$. On the other hand,

$$ABC_\alpha(S_n) = (n-1)\left(\frac{n-1}{n-2}\right)^\beta.$$

By this, the proof is complete. □

From the proof of the Theorem 3.5, we arrive at the following theorem.

Theorem 3.6. *Let T ($\neq S_n$) be a tree of order n. If $\alpha \leq -1$, then*

$$ABC_\alpha(T) \geq \frac{2}{2^\alpha} + (n-3)\left(\frac{n-3}{n-2}\right)^\alpha$$

with equality if and only if T is isomorphic to the double star $DS_{n,n-2}$.

Theorem 3.7. *Let G be a graph of order n with diameter $d \geq 4$. If $\alpha \leq -1$ then*

$$ABC_\alpha(G) \geq \frac{d-2}{2^\alpha} + \frac{\lceil (n-d+1)/2 \rceil^{\alpha+1}}{\lceil (n-d+3)/2 \rceil^\alpha} + \frac{\lfloor (n-d+1)/2 \rfloor^{\alpha+1}}{\lfloor (n-d+3)/2 \rfloor^\alpha}$$

with equality if and only if G is isomorphic to a double broom in $\mathcal{T}_{n,d}$ when $\alpha = -1$ and G is isomorphic to the balanced double broom in $\mathcal{T}_{n,d}$ when $\alpha < -1$.

Proof. Let T be any spanning tree of G and d_1 be the diameter of T. Clearly, $d_1 \geq d$. Set $\beta = -\alpha$, $a = \lceil (n-d+1)/2 \rceil$, $b = \lfloor (n-d+1)/2 \rfloor$,

$a_1 = \lceil (n-d_1+1)/2 \rceil$, and $b_1 = \lfloor (n-d_1+1)/2 \rfloor$. Then $a \geq a_1$, $b \geq b_1$ and $(a-a_1)+(b-b_1) = d_1 - d$. By Lemma 2.3 and Theorem 3.3, we have

$$\begin{aligned}
&ABC_\alpha(G) \geq ABC_\alpha(T) \\
\geq\ & \frac{d_1-2}{2^\alpha} + \frac{\lceil (n-d_1+1)/2 \rceil^{\alpha+1}}{\lceil (n-d_1+3)/2 \rceil^{\alpha}} + \frac{\lfloor (n-d_1+1)/2 \rfloor^{\alpha+1}}{\lfloor (n-d_1+3)/2 \rfloor^{\alpha}} \\
=\ & (d_1-2)\,2^\beta + \frac{(a_1+1)^\beta}{a_1^{\beta-1}} + \frac{(b_1+1)^\beta}{b_1^{\beta-1}} \\
=\ & (d-2)\,2^\beta + (a-a_1)\,2^\beta + a_1\left(\frac{a_1+1}{a_1}\right)^\beta + (b-b_1)\,2^\beta + b_1\left(\frac{b_1+1}{b_1}\right)^\beta \\
\geq\ & (d-2)\,2^\beta + (a-a_1)\left(\frac{a+1}{a}\right)^\beta + a_1\left(\frac{a+1}{a}\right)^\beta \\
& +(b-b_1)\left(\frac{b+1}{b}\right)^\beta + b_1\left(\frac{b+1}{b}\right)^\beta \\
=\ & (d-2)\,2^\beta + a\left(\frac{a+1}{a}\right)^\beta + b\left(\frac{b+1}{b}\right)^\beta \\
=\ & \frac{d-2}{2^\alpha} + \frac{\lceil (n-d+1)/2 \rceil^{\alpha+1}}{\lceil (n-d+3)/2 \rceil^{\alpha}} + \frac{\lfloor (n-d+1)/2 \rfloor^{\alpha+1}}{\lfloor (n-d+3)/2 \rfloor^{\alpha}},
\end{aligned}$$

where, in addition, we used Lemma 2.1 and $2 \geq (x+1)/x$ for $x \geq 1$. If the equality holds, then G must be a tree and by Theorem 3.3, G is isomorphic to a double broom in $\mathcal{T}_{n,d}$ when $\alpha = -1$, and G is isomorphic to the balanced double broom in $\mathcal{T}_{n,d}$ when $\alpha < -1$. □

4. Graphs of order n with k pendent vertices

Denote by $\mathcal{T}_n^k$ the set of trees of order n with k pendent vertices. Then one can easily check that $DB_{a,b,d} \in \mathcal{T}_n^k$ if $a+b = k+2$ and $a+b+d = n+3$. If $k = n-1$, then there is only one tree in $\mathcal{T}_n^{n-1}$, that is the star S_n. Therefore, we assume that $k \leq n-2$. Clearly, each tree in $\mathcal{T}_n^{n-2}$ is a double star. Hence by Theorem 3.1, we arrive at the following lemma.

Lemma 4.1. *Let T be a tree in $\mathcal{T}_n^{n-2}$ and $\alpha \leq -1$. Then*

$$ABC_\alpha(T) \geq \frac{2}{2^\alpha} + (n-3)\left(\frac{n-3}{n-2}\right)^\alpha,$$

with equality if and only if T is isomorphic to the double star $DS_{n-2,2}$.

Theorem 4.2. *Let T be a tree in $\mathcal{T}_n^k$ and $k \leq n-3$. If $\alpha \leq -1$, then*

$$ABC_\alpha(T) \geq \frac{n-k-1}{2^\alpha} + \frac{\lceil k/2 \rceil^{\alpha+1}}{\lceil (k+2)/2 \rceil^{\alpha}} + \frac{\lfloor k/2 \rfloor^{\alpha+1}}{\lfloor (k+2)/2 \rfloor^{\alpha}}, \tag{9}$$

with equality if and only if T is isomorphic to a double broom in $\mathcal{T}_n^k$ when $\alpha = -1$, and T is isomorphic to the balanced double broom in $\mathcal{T}_n^k$ when $\alpha < -1$.

Proof. For convenience, denote $\beta = -\alpha$. Let u be a maximum degree vertex in T and v be the maximum degree vertex in $V(T) \setminus \{u\}$. Also let $u_1, u_2, \ldots, u_p$ and $v_1, v_2, \ldots, v_q$ be pendent neighbors of u and v, respectively. As before, $d(u) = \Delta$ and $d(v) = \Delta_1$. Then $p \leq \Delta - 1$ and $q \leq \Delta_1 - 1$. Since T has exactly k pendent vertices, we have $\Delta + \Delta_1 \leq k + 2$ and $\Delta \geq \Delta_1 \geq 2$. For any non-pendent edge xy in T, we have

$$f_\beta(d(x), d(y)) \geq 2^\beta$$

by $d(x) \geq 2$, $d(y) \geq 2$ and Lemma 2.2. It is easy to see that if x_1y_1 is a pendent edge in T different from uu_i, $1 \leq i \leq p$ and vv_j, $1 \leq j \leq q$, then

$$f_\beta(d(x_1), d(y_1)) \geq \left(\frac{\Delta_1}{\Delta_1 - 1}\right)^\beta ,$$

by Lemma 2.2. From the above inequalities and definition of ABC_α, we have

$$\begin{aligned} ABC_\alpha(T) &\geq p\left(\frac{\Delta}{\Delta - 1}\right)^\beta + q\left(\frac{\Delta_1}{\Delta_1 - 1}\right)^\beta \\ &+ (k-p-q)\left(\frac{\Delta_1}{\Delta_1 - 1}\right)^\beta + (n-1-k)\,2^\beta \\ &= p\left[\left(\frac{\Delta}{\Delta - 1}\right)^\beta - \left(\frac{\Delta_1}{\Delta_1 - 1}\right)^\beta\right] + k\left(\frac{\Delta_1}{\Delta_1 - 1}\right)^\beta + (n-1-k)\,2^\beta \\ &\geq (\Delta-1)\left[\left(\frac{\Delta}{\Delta-1}\right)^\beta - \left(\frac{\Delta_1}{\Delta_1-1}\right)^\beta\right] + k\left(\frac{\Delta_1}{\Delta_1-1}\right)^\beta + (n-1-k)\,2^\beta \\ &= (\Delta-1)\left(\frac{\Delta}{\Delta - 1}\right)^\beta + (k-\Delta+1)\left(\frac{\Delta_1}{\Delta_1 - 1}\right)^\beta + (n-1-k)\,2^\beta \\ &\geq (\Delta-1)\left(\frac{\Delta}{\Delta - 1}\right)^\beta + (k-\Delta+1)\left(\frac{k-\Delta+2}{k-\Delta+1}\right)^\beta + (n-1-k)\,2^\beta \end{aligned}$$

since $p \leq \Delta - 1$, $(\Delta/(\Delta-1))^\beta - (\Delta_1/(\Delta_1-1))^\beta \leq 0$ and $\Delta_1 \leq k - \Delta + 2$.

If $\beta = 1$, then we get

$$ABC_\alpha(T) \geq k + 2 + 2(n-1-k) = 2n - k\,. \tag{10}$$

If the equality in (10) holds, then clearly $\Delta + \Delta_1 = k + 2$ and it follows that any pendent vertex in T is adjacent to either u or v. Let P be the path from u to v. Then a degree of any vertex on P, different from u and v, is 2. Namely, if it were greater than 2, then there would exists a pendent vertex that is not adjacent to u and v. Hence, T is isomorphic to a double broom in $\mathcal{T}_n^k$. Conversely, if T is isomorphic to a double broom in $\mathcal{T}_n^k$, then the diameter of T is $n - k + 1$. Then by Lemma 3.2, we have

$$ABC_{-1}(T) = n + (n-k+1) - 1 = 2n - k\,.$$

If $\beta > 1$ then by Lemma 2.6, we have

$$\begin{aligned} ABC_\alpha(T) &\geq 2^\beta(n-k-1) + \frac{\Delta^\beta}{(\Delta-1)^{\beta-1}} + \frac{(k-\Delta+2)^\beta}{(k-\Delta+1)^{\beta-1}} \\ &\geq 2^\beta(n-k-1) + \frac{\lceil (k+2)/2 \rceil^\beta}{\lceil k/2 \rceil^{\beta-1}} + \frac{\lfloor (k+2)/2 \rfloor^\beta}{\lfloor k/2 \rfloor^{\beta-1}} \quad (11) \\ &= \frac{n-k-1}{2^\alpha} + \frac{\lceil k/2 \rceil^{\alpha+1}}{\lceil (k+2)/2 \rceil^\alpha} + \frac{\lfloor k/2 \rfloor^{\alpha+1}}{\lfloor (k+2)/2 \rfloor^\alpha}. \end{aligned}$$

Suppose now that equality in (9) holds. Then $\Delta + \Delta_1 = k+2$ and it follows that T is isomorphic to a double broom in $\mathcal{T}_n^k$. Also the equality in (11) holds. Hence, we have $\Delta = \lceil (k+2)/2 \rceil$ and $\Delta_1 = \lfloor (k+2)/2 \rfloor$. Therefore, T is isomorphic to the balanced double broom in $\mathcal{T}_n^k$. Conversely, if T is isomorphic to the balanced double broom in $\mathcal{T}_n^k$, then one can easily see that the equality in (9) holds. □

Corollary 4.3. [16] *Let T be a tree in $\mathcal{T}_n^k$ and $k \leq n-3$. Then*

$$AZI(T) \geq 8(n-k-1) + \frac{\lceil (k+2)/2 \rceil^3}{\lceil k/2 \rceil^2} + \frac{\lfloor (k+2)/2 \rfloor^3}{\lfloor k/2 \rfloor^2},$$

with equality if and only if T is isomorphic to the balanced double broom in $\mathcal{T}_n^k$.

Theorem 4.4. *Let G be a graph of order n with k cut edges. If $k \leq n-3$ and $\alpha \leq -1$, then*

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

with equality if and only if G is isomorphic to the graph obtained from C_{n-k} by attaching k pendent vertices to one vertex of C_{n-k}.

Proof. Let m be the number of edges of G. Since $k \leq n-3$, G is not isomorphic to a tree and it follows that $m \geq n$. If $m > n$, then there exist at least $n-k+1$ non-pendent edges in G. Therefore,

$$\begin{aligned} ABC_\alpha(G) &\geq \frac{n-k+1}{2^\alpha} + k \cdot \left(\frac{\Delta-1}{\Delta}\right)^\alpha \\ &\geq \frac{n-k}{2^\alpha} + 2^{-\alpha} + k \cdot \left(\frac{n-1}{n-2}\right)^{-\alpha} \\ &\geq \frac{n-k}{2^\alpha} + (k+1)\left(\frac{2+k(n-1)/(n-2)}{k+1}\right)^{-\alpha} \\ &> \frac{n-k}{2^\alpha} + k\left(\frac{k+2}{k+1}\right)^{-\alpha} = \frac{n-k}{2^\alpha} + k\left(\frac{k+1}{k+2}\right)^\alpha \quad (12) \end{aligned}$$

since Lemma 2.5, $(n-1)/(n-2) > 1$ and $\alpha \leq -1$. Thus, G is unicyclic. Then, it is easy to see that $\Delta \leq k+2$. Since there exist exactly $n-k$ non-pendent edges in G, we have

$$ABC_\alpha(G) \geq \frac{n-k}{2^\alpha} + k \cdot \left(\frac{\Delta-1}{\Delta}\right)^\alpha \geq \frac{n-k}{2^\alpha} + k\left(\frac{k+1}{k+2}\right)^\alpha \quad (13)$$

and the equality holds if and only if G is isomorphic to the graph obtained from C_{n-k} by attaching k pendent vertices to one vertex of C_{n-k}. □

Theorem 4.5. *Let G be a unicyclic graph of order n with girth g. If $\alpha < 0$ then*

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

with equality if and only if G is isomorphic to the graph obtained from C_g by attaching $n-g$ pendent vertices to one vertex of C_g.

Proof. Since the number of cut edges in G is $n-g$ and the extremal graph in Theorem 4.4 is unicyclic, we get the required result by Theorem 4.4. □

The same argument as in the proof of Theorem 4.4 yields the following result.

Theorem 4.6. *Let G be a cyclic graph of order n with k pendent vertices and $0 \leq k \leq n-3$. If $\alpha \leq -1$, then*

$$ABC_\alpha(G) \geq \frac{n-k}{2^\alpha} + k\left(\frac{k+1}{k+2}\right)^\alpha.$$

with equality if and only if G is isomorphic to the graph obtained from C_{n-k} by attaching k pendent vertices to one vertex of C_{n-k}.

Acknowledgment. The authors thank the anonymous reviewers for their helpful suggestions. B. Horoldagva is thankful for the support of the Mongolian National University of Education.

References

[1] A. Ali, K.C. Das, D. Dimitrov, B. Furtula, *Atom-bond connectivity index of graphs: A review over extremal results and bounds*, Discrete Math. Lett. **5** (2021), 68–93.
[2] A. Ali, B. Furtula, I. Gutman, D. Vukičević, *Augmented Zagreb index: Extremal results and bounds*, MATCH Commun. Math. Comput. Chem. **85** (2021), 221–244.
[3] C. Chen, M. Liu, X. Chen, W. Lin, *On general ABC-type index of connected graphs*, Discrete Appl. Math. **315** (2022), 27–35.
[4] X. Chen, K.C. Das, *Solution to a conjecture on the maximum ABC index of graphs with given chromatic number*, Discrete Appl. Math. **251** (2018), 126–134.
[5] X. Chen, G. Hao, *Extremal graphs with respect to generalized ABC index*, Discrete Appl. Math. **243** (2018), 115–124.
[6] K.C. Das, S. Elumalai, I. Gutman, *On ABC index of graphs*, MATCH Commun. Math. Comput. Chem. **78** (2017), 459–468.
[7] K.C. Das, J.M. Rodríguez, J.M. Sigarreta, *On the maximal general ABC index of graphs with given maximum degree*, Appl. Math. Comput. **386** (2020), #125531.
[8] K.C. Das, J.M. Rodríguez, J.M. Sigarreta, *On the generalized ABC index of graphs*, MATCH Commun. Math. Comput. Chem. **87** (2022), 147–169.
[9] D. Dimitrov, Z. Du, *Complete characterization of the minimal-ABC trees*, Discrete Appl. Math. **336** (2023), 148–194.
[10] D. Dimitrov, Z. Du, *The ABC index conundrum's complete solution*, MATCH Commun. Math. Comput. Chem. **91** (2024), 000–000.
[11] E. Estrada, *Atom-bond connectivity and the energetic of branched alkanes*, Chem. Phys. Lett. **463** (2008), 422–425.
[12] 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.
[13] B. Furtula, A. Graovac, D. Vukičević, *Augmented Zagreb index*, J. Math. Chem. **48** (2010), 370–380.
[14] I. Gutman, I., J. Tošović, S. Radenković, S.Marković, *On atom–bond connectivity index and its chemical applicability*, Indian J. Chem. **51A** (2012), 690–694.
[15] Y. Huang, *Trees with given diameter minimizing the augmented Zagreb index and maximizing the ABC index*, Commun. Math. Res. **33** (2017), 8–18.
[16] Y. Huang, B. Liu, *Ordering graphs by the augmented Zagreb indices*, J. Math. Res. Appl. **35** (2015), 119–129.
[17] Y. Huang, B. Liu, L. Gan, *Augmented Zagreb index of connected graphs*, MATCH Commun. Math. Comput. Chem. **67** (2012), 483–494.
[18] W. Lin, A. Ali, H. Huang, Z. Wu, J. Chen, *On the trees with maximal augmented Zagreb index*, IEEE Access **6** (2018), 69335–69341.
[19] W. Lin, D. Dimitrov, R. Škrekovski, *Complete characterization of trees with maximal augmented Zagreb index*, MATCH Commun. Math. Comput. Chem. **83** (2020), 167–178.
[20] K.N. Prakasha, P.S.K. Reddy, I.N. Cangul, *Atom-bond-connectivity index of certain graphs*, TWMS J. Appl. Eng. Math. **13** (2023), 400–408.
[21] Z. Shao, P. Wu, Y. Gao, I. Gutman, X. Zhang, *On the maximum ABC index of graphs without pendent vertices*, Appl. Math. Comput. **315** (2017), 298–321.

[22] Z. Shao, P. Wu, H. Jiang, S.M. Sheikholeslami, S. Wang, *On the maximum ABC index of bipartite graphs without pendent vertices*, Open Chem. **18** (2020), 39–49.

[23] X. Wu, L. Zhang, *On structural properties of ABC-minimal chemical trees*, Appl. Math. Comput. **362** (2019), #124570.

[24] X. Zhang, Y. Sun, H. Wang, X. Zhang, *On the ABC index of connected graphs with given degree sequences*, J. Math. Chem. **56** (2018), 568–582.