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Complete Characterization of Trees with Maximal Augmented Zagreb Index*

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Abstract

The augmented Zagreb index (AZI) of an n-vertex graph $G = (V, E)$ is defined as $AZI(G) = \sum_{v_i v_j \in E} [d_i d_j/(d_i + d_j - 2)]^3$, where $V = \{v_0, v_1, \cdots, v_{n-1}\}$, $n \geq 3$, and d_i denotes the degree of vertex v_i of G. As a variant of the well-known atom-bond connectivity index, the AZI was shown to have the best predicting ability for a variety of physicochemical properties among several tested vertex-degree-based topological indices. In 2010 Furtula et al. [J. Math. Chem. 48 (2010) 370] proposed the problem of characterizing n-vertex tree(s) with maximal AZI. In the present paper we solve this problem by proving that the n-vertex balanced double star uniquely maximizes AZI if $n \geq 19$.

1 Introduction

We consider connected simple graphs with at least 3 vertices only. Such a graph will be denoted by $G = (V, E)$, where $V = V(G) = \{v_0, v_1, \cdots, v_{n-1}\}$ and $E = E(G)$ are the vertex set and edge set of G, respectively. Let $d_i = d(v_i)$ denote the degree of vertex v_i, and $\Delta = \Delta(G)$ the maximum degree of G. A chemical graph is a graph with $\Delta \leq 4$. The sequence $\pi = \pi(G) = (d_0, d_1, \cdots, d_{n-1})$ is called the degree sequence of G. In particular,

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if G is a tree, then π is called a tree degree sequence. Let $\boldsymbol{C}(\pi) = \{G|G$ is connected and $\pi(G) = \pi\}$, and $\boldsymbol{T}(\pi) = \{T|T$ is a tree and $\pi(T) = \pi\}$.

The atom-bond connectivity (ABC) index of a graph $G = (V, E)$ was defined [1] as $ABC(G) = \sum_{v_iv_j \in E} \sqrt{(d_i + d_j - 2)/(d_i d_j)}$. This topological index turned out to be closely correlated with the heat of formation of alkanes, and a quantum-chemical explanation for its descriptive ability was provided in [2]. Gutman et al. [3] later confirmed that the ABC index could reproduce the heat of formation with accuracy comparable to that of high-level ab initio and DFT (MP2, B3LYP) quantum chemical calculations. Due to these applications, there is an increased interest in the mathematical properties of the ABC index in the last few years (see [4-27, 48, 49]). However, the following elementary problem remains open and was coined [14] as the "ABC index conundrum".

Problem A. Characterize n-vertex tree(s) with minimal ABC index.

On the other hand, in order to explore better correlation abilities of the ABC index for the heat of formation of alkanes, Furtula et al. [28] made a generalization of this index by replacing the exponent 1/2 with an arbitrary non-zero real number $-\lambda$. Namely, they defined $ABC_\lambda(G) = \sum_{v_iv_j \in E} [(d_i + d_j - 2)/(d_i d_j)]^{-\lambda}$, and showed the so-called augmented Zagreb index $AZI = ABC_3$ is better than ABC index in predicting the heat of formation of octanes and heptanes. Moreover, in 2013 some experiments [29, 30] showed that, the AZI has the best predicting ability for a variety of physicochemical properties among several tested vertex-degree-based topological indices. Consequently, some researchers initiated the study of the mathematical properties of AZI. Furtula et al. [28] proved that the star is the unique tree having the minimal AZI among n-vertex trees. Some upper and lower bounds for the AZI of connected graphs were reported in [31] and [32]. Zhan et al. [33] determined the n-vertex unicyclic graphs with minimal and second minimal AZI, as well as the n-vertex bicyclic graphs with minimal AZI. Huang and Liu [34] considered the ordering of n-vertex connected graphs, trees, unicyclic graphs, and bicyclic graphs with respect to AZI. In [35] and [36] some bounds for the AZI of catacondensed polyomino and/or hexagonal chains and/or systems were obtained. The AZI of fluoranthene-type benzenoid systems were considered in [37] and [38]. Ali et al. [39] characterized the extremal graphs with maximal AZI among n-vertex connected graphs with given vertex connectivity or matching number, and determined [40] the graphs with minimal AZI among n-vertex cacti with given number of cycles. Palacios [41] gave a lower bound of

AZI in terms of numbers of vertices and edges, and the maximum degree of a graph. Ali et al. [42] reported some tight bounds for the AZI of chemical unicyclic and bicyclic graphs, as well as an Nordhaus-Gaddum-type result. Sun et al. [43] established some lower bounds for the AZI of trees and unicyclic graphs with perfect matchings. Recently, Chen and Hao [44] characterized the graphs with maximal $ABC_\lambda(G)$ value for $\lambda > 0$ among n-vertex connected graphs with given vertex connectivity, edge connectivity, or matching number. It needs to be mentioned here that, the definition of the generalized ABC index of a graph $G = (V, E)$ they used is $ABC_\alpha(G) = \sum_{v_iv_j \in E} [(d_i + d_j - 2)/(d_i d_j)]^\alpha$.

However, as the counterpart of Problem A, the following elementary problem proposed by Furtula et al. [28] in 2010 remains open.

Problem B. Characterize n-vertex tree(s) with maximal AZI.

Ali et al. [39] did the first work on this problem. They showed that, n-vertex tree(s) with maximal AZI share some structural properties with those with minimal ABC index. Recently, Lin et al. [45] made a solid step towards the problem. Firstly it was showed that, given a degree sequence π there is a so-called BFS graph with maximal AZI in $\boldsymbol{C}(\pi)$. This allows them conducted a computer search for n-vertex tree(s) with maximal AZI up to $n = 200$. Based on the search results (see the Table 1 in [45]) they proposed the following conjecture.

Conjecture 1.1 [45]**.** If $n \geq 19$, $D(n; \lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor)$ (the balanced double star, see Figure. 1) is the unique n-vertex tree with maximal AZI.

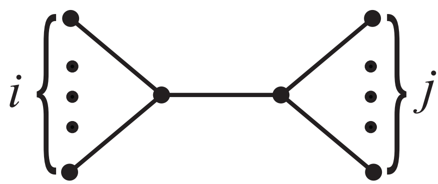

Figure 1. The double star $D(n; i, j)$, $i + j = n - 2$

Moreover, towards this conjecture Lin et al. [45] showed that, an n-vertex tree with maximal AZI has no vertices of degree 2 if $n \geq 19$. In the present paper, we will confirm this conjecture, namely, will completely solve Problem B.

2 Some properties of $[xy/(x+y-2)]^3$

For $x, y \geq 1$ with $x+y \geq 3$ let $h(x,y) = [xy/(x+y-2]^3$, and for $x \geq 2$ and $y \geq 1$ with $x+y \geq 4$ let $l(x,y) = h(x,y) - h(x-1,y)$. Since $AZI(G)$ is just the sum of $h(d_i, d_j)$ over all pairs of adjacent vertices v_i and v_j of G, it is purposeful to establish some properties of $h(x,y)$.

Lemma 2.1 [32]**.**

(1) $h(x,1)$ strictly decreases with $x \geq 2$.

(2) $h(x,2) = 8$.

(3) If $y \geq 3$ is fixed, then $h(x,y)$ strictly increases with $x \geq 2$.

Lemma 2.2 [45]**.** If $x, y, z \geq 3$ and $w \geq 2$, then

$$1 < h(z,1) \leq h(3,1) = (3/2)^3 < h(2,1) = h(2,w) = 8 < (9/4)^3 = h(3,3) \leq h(x,y),$$

with the equalities iff $z = 3$ and $x = y = 3$, respectively.

Lemma 2.3 [45] **.** $l(x,y+1) > l(x,y)$ for $x \geq 2$ and $y \geq 1$ with $x+y \geq 4$.

Lemma 2.4 [45] **.** For $x \geq 2$ and $y \geq 1$,

(1) $l(x,1)$ (< 0) strictly increases with $x \geq 3$.

(2) $l(x,2) = 0$ for $x \geq 3$.

(3) If $y \geq 3$ is fixed, then $l(x,y)$ (> 0) strictly increases with $2 \leq x \leq y-1$, and strictly decreases with $x \geq y$.

Lemma 2.5. If $y > x \geq 2$, then $l(x,y) > l(y,x)$. Hence $h(x+1, y-1) > h(x,y)$ if $y \geq x+2 \geq 3$.

Proof. From Lemmas 2.3 and 2.4 we have $l(x,y) \geq l(x,x+1) > l(x,x) > l(y,x)$. Hence

$$h(x+1, y-1) - h(x,y) = l(x+1,y) - l(y,x+1) > 0. \qquad \blacksquare$$

Lemma 2.6. Let $x \geq 3$ and $f(x) = (x-2)l(x,1) + h(x,1)$. Then $f(x)$ strictly increases with x, and $-1.25 \leq f(x) < 1$.

Proof. Let $g(x) = (x-1)h(x,1)$. It is easily seen that $g'(x) = [x^3/(x-1)^2]' = x^2(x-3)/(x-1)^3$, and so $g''(x) = 6x/(x-1)^4 > 0$. Hence $g(x)$ is strictly convex in $[2, +\infty)$. It follows that $f(x) = (x-1)h(x,1) - (x-2)h(x-1,1) = g(x) - g(x-1)$ strictly increases with $x \geq 3$. Immediately we have $f(x) \geq f(3) = -1.25$.

To prove $f(x) < 1$, it suffices to show $\lim_{x \to +\infty} f(x) = 1$, which is easily seen from

$$f(x) = \frac{x^3}{(x-1)^2} - \frac{(x-1)^3}{(x-2)^2} = \frac{x^4 - 6x^3 + 10x^2 - 5x + 1}{x^4 - 6x^3 + 13x^2 - 12x + 4}.$$

The proof is thus completed. ■

Lemma 2.7. If $x \geq 3$, then $(x-2)l(x,1) \geq -4.625$.

Proof. From Lemmas 2.2 and 2.6 we have

$$(x-2)l(x,1) \geq -1.25 - h(x,1) \geq -1.25 - h(3,1) = -4.625. \qquad \blacksquare$$

Lemma 2.8 [45] **.** $l(y+1,y)$ strictly increases with $y \geq 4$.

Lemma 2.9. $h(y+1,y+1)+h(y-2,y) > 2h(y,y) > h(y+1,y)+h(y-1,y)$ if $y \geq 4$.

Proof. By elementary computations we have

$$h(y+1,y+1)+h(y-2,y) > 2h(y,y) \Leftrightarrow \frac{(y+1)^6}{(2y)^3} + \frac{y^3(y-2)^3}{[2(y-2)]^3} > 2\frac{y^6}{[2(y-1)]^3}$$

$$\Leftrightarrow 3y^7 - 9y^6 - 6y^5 + 6y^4 + 8y^3 - 3y - 1 > 0$$

$$\Leftarrow 3y^5(y^2 - 3y - 2) > 0$$

$$\Leftarrow y \geq 4.$$

On the other hand, from Lemma 2.4 we have $l(y,y) > l(y+1,y)$, and the second part follows immediately. ■

Lemma 2.10. $yl(y+1,y-1) \geq (y-3)l(y-1,y)$ if $y \geq 3$, with the equality iff $y = 3$.

Proof. The conclusion holds obviously if $y = 3$, hence assume $y \geq 4$. By elementary computations we have

$$\begin{aligned} yl(y+1,y-1) &= y(y-1)^3[\frac{(y+1)^3}{(2y-2)^3} - \frac{y^3}{(2y-3)^3}] \\ &= y(y-1)^3[\frac{y+1}{2y-2} - \frac{y}{2y-3}][(\frac{y+1}{2y-2})^2 + \frac{y(y+1)}{(2y-2)(2y-3)} + (\frac{y}{2y-3})^2] \\ &> 3y(y-1)^3\frac{y-3}{(2y-2)(2y-3)}(\frac{y}{2y-3})^2 \\ &= \frac{3(y-3)(y-1)^2y^3}{2(2y-3)^3}. \end{aligned}$$

Analogously we have $l(y-1,y) < 3(y-1)^2y^3/[2(2y-3)^3]$, and the conclusion follows immediately. ■

3 Main results

To prove Conjecture 1.1 we need more preliminaries. For convenience, we call an n-vertex tree with maximal AZI is optimal. If π is the degree sequence of an optimal tree, then π is said to be an optimal tree degree sequence. In this section we always assume: (1) $n \geq 19$; (2) $\pi = (\Delta = d_0, d_1, \cdots, d_t, 1^{n-t-1})$ is a non-increasing optimal tree degree sequence, where $d_t \geq 2$ and 1^k denotes k successive 1's; and (3) T is the (unique) greedy (rooted) tree in $\boldsymbol{T}(\pi)$. For the concepts and properties of the so-called BFS graphs and greedy trees, one can refer to [46] and [47].

From the Lemmas 20-22 and the Theorem 23 in [45], we conclude some features of an optimal tree degree sequence π and the corresponding greedy tree T.

Lemma 3.1 [45] **.** $t \geq 1$, $\Delta \geq 10$, and $d_t \geq 3$.

Lemma 3.2. If $t \geq 2$, $1 \leq \tau \leq t-1$, and p is the parent of v_τ, then $d_\tau \geq d(p) - 1$.

Proof. By contradiction suppose $d_\tau \leq d(p) - 2$. Let u be the parent of v_t, and w a child of v_t. Let $T_1 = T - v_t w + v_\tau w$. For convenience let $x = d_t$, $y = d_\tau$, $z = d(u)$, and $r = d(p)$. y_i's, $i = 1, 2, \cdots, y-1$, will denote the degrees of the children of v_τ. The degree of u in T_1 is $z+1$ or z, depending on if $u = v_\tau$ or not. Since T is greedy, we have $r \geq z$ and $r - 2 \geq y \geq x \geq 3$. From Lemmas 2.2-2.4 and 2.6 we have

$$\begin{aligned}
AZI(T_1) - AZI(T) &\geq h(y+1, r) + h(x-1, z) + (x-2)h(x-1, 1) + h(y+1, 1) \\
&\quad + \sum_{i=1}^{y-1} h(y+1, y_i) - [h(y, r) + h(x, z) + (x-1)h(x, 1) \\
&\quad + \sum_{i=1}^{y-1} h(y, y_i)] \quad (Lemma\ 2.2) \\
&\geq l(y+1, r) - l(x, z) + [(y-1)l(y+1, 1) + h(y+1, 1)] \\
&\quad - [(x-2)l(x, 1) + h(x, 1)] \quad (Lemma\ 2.3) \\
&> l(y+1, r) - l(y, r) \quad (Lemmas\ 2.3,\ 2.4,\ 2.6) \\
&> 0, \quad (y \leq r-2 \ and\ Lemma\ 2.4)
\end{aligned}$$

a contradiction. The proof is thus completed. ■

Lemma 3.3. $t \leq \Delta$.

Proof. Suppose $t > \Delta$. Let u be the parent of v_t, and w a child of v_t. Let $T_1 = T - v_t w + v_0 w$. For convenience let $x = d_t$, $y = d_0 = \Delta$, and $z = d(u)$. Let y_i's, $i = 1, 2, \cdots, y$, denote the degrees of the children of v_0. From Lemmas 3.1 and 3.2 we have $y_\Delta \geq y - 1 \geq 9$. In addition we have $y \geq z \geq x$ since T is greedy. From Lemmas 2.2-2.4 and 2.6 we have

$$\begin{aligned}
AZI(T_1) - AZI(T) &= \sum_{i=1}^{y} h(y+1, y_i) + h(y+1, 1) + h(x-1, z) + (x-2)h(x-1, 1) \\
&\quad - [\sum_{i=1}^{y} h(y, y_i) + h(x, z) + (x-1)h(x, 1)] \\
&\geq yl(y+1, y-1) - l(x, z) + h(y+1, 1) \\
&\quad - [(x-2)l(x, 1) + h(x, 1)] \quad (Lemma\ 2.3)
\end{aligned}$$

$$> yl(y+1,y-1) - l(y-1,y) \quad (Lemmas\ 2.2-2.4\ and\ 2.6)$$
$$> 0, \quad (y \geq 10\ and\ Lemma\ 2.10)$$

a contradiction. The proof is thus completed. ■

Now we are in the position to prove Conjecture 1.1.

Proof of Conjecture 1.1. For convenience let $z = d_0$, $y = d_1$, and $x = d_2$. From Lemmas 3.1 and 3.3 we have $1 \leq t \leq \Delta$. Hence all children of v_i, $1 \leq i \leq t$, are pendent vertices. We distinguish the following two cases.

Case 1. $t = 1$. Then $T = D(n; z-1, y-1)$. If $T \neq D(n; \lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor)$, then $z - 2 \geq y \geq 3$. Let $T_1 = D(n; z-2, y)$. From Lemmas 2.3, 2.4, and 2.6 we have

$$\begin{aligned}
AZI(T_1) - AZI(T) &= h(y+1, z-1) + yh(y+1,1) + (z-2)h(z-1,1) \\
&\quad - [h(y,z) + (y-1)h(y,1) + (z-1)h(z,1)] \\
&= [h(y+1,z-1) - h(y,z)] + [(y-1)l(y+1,1) + h(y+1,1)] \\
&\quad - [(z-2)l(z,1) + h(z,1)] \\
&> l(y+1,z-1) - l(z,y) - 1.25 - 1 \quad (Lemma\ 2.6) \\
&\geq l(y+1,y+1) - l(y+2,y) - 2.25 \quad (Lemmas\ 2.3\ and\ 2.4) \\
&= h(y+1,y+1) - h(y+2,y) - 2.25 \\
&= [(y+1)^6 - y^3(y+2)^3]/(8y^3) - 2.25 \\
&= [3y^4 + 12y^3 + 15y^2 + 6y + 1]/(8y^3) - 2.25 \\
&> (3y+12)/8 - 2.25 \\
&\geq 0.375, \quad (y \geq 3)
\end{aligned}$$

contradicting that T is optimal.

Case 2. $t \geq 2$. Then $z \geq y \geq x \geq 3$ and $y \geq z-1 \geq 9$ from Lemmas 3.1 and 3.2. Denote the degrees of the children of v_0 by z_i's, $1 \leq i \leq z$. Note that $z_1 = y$ and $z_2 = x$. Let u_1 and u_2 be two children of v_2, and $T_1 = T - v_2u_1 - v_2u_2 + v_0u_1 + v_1u_2$.

Subcase 2.1. $z = y + 1$. From Lemmas 2.2-2.8 we have

$$\begin{aligned}
AZI(T_1) - AZI(T) &= h(x-2, y+2) + h(y+1, y+2) + \sum\nolimits_{i=3}^{y+1} h(y+2, z_i) + h(y+2, 1) \\
&\quad + yh(y+1,1) + (x-3)h(x-2,1) - [h(x,y+1) + h(y,y+1) \\
&\quad + \sum\nolimits_{i=3}^{y+1} h(y+1, z_i) + (y-1)h(y,1) + (x-1)h(x,1)]
\end{aligned}$$

$$\geq [h(x-2,y+2)+h(y+1,y+2)-h(x,y+1)-h(y,y+1)]$$
$$+(y-1)l(y+2,1)+(x-3)[h(x-2,1)-h(x,1)]+h(y+2,1)$$
$$+[(y-1)l(y+1,1)+h(y+1,1)]-2h(x,1) \quad (Lemma\ 2.3)$$
$$> [h(x-2,y+2)+h(y+1,y+2)-h(x,y+1)-h(y,y+1)]$$
$$+(y-1)l(y+1,1)+1-1.25-2h(3,1) \quad (Lemmas\ 2.2,\ 2.4,\ 2.6)$$
$$> h(x,y)-h(x,y+1)+h(y+1,y+2)$$
$$-h(y,y+1)]-11.625 \quad (Lemmas\ 2.5\ and\ 2.7)$$
$$= l(y+2,y+1)+[l(y+1,y+1)-l(y+1,x)]-11.625$$
$$> l(y+2,y+1)-11.625 \quad (Lemma\ 2.3)$$
$$\geq l(11,10)-11.625 \quad (y\geq 9\ and\ Lemma\ 2.8)$$
$$= 10.9588.$$

Hence $AZI(T) < AZI(T_1)$, a contradiction.

Subcase 2.2. $z = y$ (≥ 10). From Lemmas 2.2-2.9 we have

$$AZI(T_1)-AZI(T) = h(x-2,y+1)+h(y+1,y+1)+\sum_{i=3}^{y} h(y+1,z_i)+h(y+1,1)$$
$$+yh(y+1,1)+(x-3)h(x-2,1)-[h(x,y)+h(y,y)$$
$$+\sum_{i=3}^{y} h(y,z_i)+(y-1)h(y,1)+(x-1)h(x,1)]$$
$$\geq h(x-2,y+1)+h(y+1,y+1)-h(x,y)-h(y,y)$$
$$+(y-2)l(y+1,1)+(x-3)[h(x-2,1)-h(x,1)]+h(y+1,1)$$
$$+[(y-1)l(y+1,1)+h(y+1,1)]-2h(x,1) \quad (Lemma\ 2.3)$$
$$> h(x-2,y+1)+h(y+1,y+1)-h(x,y)-h(y,y)$$
$$+(y-2)l(y,1)+1-1.25-2h(3,1) \quad (Lemmas\ 2.2\ and\ 2.6)$$
$$> h(x-1,y)+h(y+1,y+1)$$
$$-h(x,y)-h(y,y)-11.625 \quad (Lemmas\ 2.5\ and\ 2.7)$$
$$= -l(x,y)+l(y+1,y+1)+l(y+1,y)-11.625$$
$$> -l(y-1,y)+l(y+1,y+1)+l(y+1,y)-11.625 \quad (Lemma\ 2.4)$$
$$= h(y+1,y+1)+h(y-2,y)-[h(y,y+1)+h(y-1,y)]$$
$$+l(y+1,y)-11.625$$
$$> l(11,10)-11.625 \quad (y\geq 10\ and\ Lemmas\ 2.8\ and\ 2.9)$$

$$= 10.9588.$$

Hence $AZI(T) < AZI(T_1)$, again a contradiction.

The proof is thus completed. ■

4 Discussions

It is interesting that, among n-vertex trees ($n \geq 19$) the star $K_{1,n-1}$ uniquely minimizes the AZI, while the balanced double star $D(n; \lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor)$ uniquely maximizes the AZI. Both $K_{1,n-1}$ and $D(n; \lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor)$ have many pendent vertices, and both their diameters are small. It may be worthy of investigating the change of the AZI of a tree when it evaluates from $K_{1,n-1}$ to $D(n; \lceil \frac{n-2}{2} \rceil, \lfloor \frac{n-2}{2} \rfloor)$. Another, it is easily known that, among n-vertex connected graphs the complete graph K_n uniquely maximizes the AZI. However, which graph(s) have maximal AZI among (m, n)-graphs (connected graphs with n vertices and m edges) for $m \geq n$? Therefore the following problems may be interesting.

Promblem 4.1. Characterize extremal trees with given diameter.

Promblem 4.2. Characterize extremal trees with given number of leaves.

Promblem 4.3. Order trees by their AZI.

Promblem 4.4. Characterize extremal (m, n)-graphs for $m \geq n$.

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