

Ordering Graphs by the Augmented Zagreb Indices

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Abstract Recently, Furtula et al. proposed a valuable predictive index in the study of the heat of formation in octanes and heptanes, the augmented Zagreb index (AZI index) of a graph G , which is defined as

$$\text{AZI}(G) = \sum_{uv \in E(G)} \left(\frac{d_u d_v}{d_u + d_v - 2} \right)^3,$$

where $E(G)$ is the edge set of G , d_u and d_v are the degrees of the terminal vertices u and v of edge uv , respectively. In this paper, we obtain the first five largest (resp., the first two smallest) AZI indices of connected graphs with n vertices. Moreover, we determine the trees of order n with the first three smallest AZI indices, the unicyclic graphs of order n with the minimum, the second minimum AZI indices, and the bicyclic graphs of order n with the minimum AZI index, respectively.

Keywords augmented Zagreb index; connected graphs; trees; unicyclic graphs; bicyclic graphs

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1. Introduction

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. Let $n = |V(G)|$ and $m = |E(G)|$. Let $N(u)$ be the set of all neighbors of $u \in V(G)$ in G , and let $d_u = |N(u)|$ be the degree of vertex u . A vertex u is called a pendent vertex if $d_u = 1$. A connected graph G is called a tree (resp., unicyclic graph and bicyclic graph) if $m = n - 1$ (resp., $m = n$ and $m = n + 1$).

Molecular descriptors have found a wide application in QSPR/QSAR studies [1]. Among them, topological indices have a prominent place. Inspired by recent work on the atom-bond connectivity index [2,3], Furtula et al. [4] proposed a valuable predictive index whose prediction power is better than atom-bond connectivity index in the study of the heat of formation in octanes and heptanes, the augmented Zagreb index (AZI index for short) of a graph G , which is defined as

$$\text{AZI}(G) = \sum_{uv \in E(G)} \left(\frac{d_u d_v}{d_u + d_v - 2} \right)^3.$$

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Basic properties of AZI index have been studied in [5]. Besides, by using different graph parameters, some attained upper and lower bounds and the corresponding extremal graphs on the AZI indices for various classes of connected graphs have been given in [4,5].

In this paper, we obtain the first five largest (resp., the first two smallest) AZI indices of connected graphs with n vertices. Moreover, we determine the trees of order n with the first three smallest AZI indices, the unicyclic graphs of order n with the minimum, the second minimum AZI indices, and the bicyclic graphs of order n with the minimum AZI index, respectively.

2. The first five largest AZI indices of connected graphs

Denote by P_n , C_n , K_n and S_n the path, cycle, complete graph and star of order n , respectively. Let $G_1 \vee G_2$ denote the graph obtained from two graphs G_1 and G_2 by connecting the vertices of G_1 with the vertices of G_2 . Let \overline{G} be the complement of a graph G . Let $G + e$ denote the graph obtained from a graph G by inserting an edge $e \notin E(G)$. Let $G - e$ denote the graph obtained from a graph G by deleting the edge $e \in E(G)$. Let $S_n^+ = S_n + e$.

Let \mathbb{G}_n be the set of connected graphs of order n , and let $\mathbb{G}_{n,m}$ be the set of connected graphs with n vertices and m edges, where $n - 1 \leq m \leq \binom{n}{2}$. Obviously, $\mathbb{G}_1 = \{K_1\}$, $\mathbb{G}_2 = \{K_2\}$ and $\mathbb{G}_n = \cup_{n-1 \leq m \leq \binom{n}{2}} \mathbb{G}_{n,m}$. Now we shall investigate the AZI index of $G \in \mathbb{G}_n$ for $n \geq 3$. To begin with, a key lemma to obtain our main results is given as follows.

Lemma 2.1 ([5]) *Let $G \in \mathbb{G}_n$ and $G \not\cong K_n$, where $n \geq 3$. Then for $e \notin E(G)$, $\text{AZI}(G) < \text{AZI}(G + e)$.*

It follows from Lemma 2.1 that

Corollary 2.2 *Let n, m_1, m_2 be integers with $n \geq 3$ and $n - 1 \leq m_1 < m_2 \leq \binom{n}{2}$.*

(1) *Let $G_1 \in \mathbb{G}_{n,m_1}$. Then there exists a graph $G_2 \in \mathbb{G}_{n,m_2}$ such that $\text{AZI}(G_2) > \text{AZI}(G_1)$.*

(2) *Let $G_2 \in \mathbb{G}_{n,m_2}$. Then there exists a graph $G_1 \in \mathbb{G}_{n,m_1}$ such that $\text{AZI}(G_1) < \text{AZI}(G_2)$.*

Observe that $\mathbb{G}_3 = \{K_3, P_3\}$ and $\mathbb{G}_4 = \{K_4, K_4 - e, C_4, S_4^+, P_4, S_4\}$. By Corollary 2.2 and simply calculating, we immediately get $\text{AZI}(K_3) > \text{AZI}(P_3)$ and

$$\text{AZI}(K_4) > \text{AZI}(K_4 - e) > \text{AZI}(C_4) > \text{AZI}(S_4^+) > \text{AZI}(P_4) > \text{AZI}(S_4).$$

For $n \geq 5$, observe that $\mathbb{G}_{n,\binom{n}{2}} = \{K_n\}$, $\mathbb{G}_{n,\binom{n}{2}-1} = \{K_n - e\}$, $\mathbb{G}_{n,\binom{n}{2}-2} = \{\overline{S_3} \vee K_{n-3}, C_4 \vee K_{n-4}\}$ and $\mathbb{G}_{n,\binom{n}{2}-3} = \{\overline{S_4} \vee K_{n-4}, \overline{K_3} \vee K_{n-3}, P_4 \vee K_{n-4}, \overline{S_3} \vee (K_{n-3} - e), C_4 \vee (K_{n-4} - e) (n \geq 6)\}$.

Lemma 2.3 *Let $G \in \mathbb{G}_{n,\binom{n}{2}-3}$ and $G \not\cong \overline{S_4} \vee K_{n-4}$. Then for $n \geq 5$,*

$$\text{AZI}(\overline{S_3} \vee K_{n-3}) > \text{AZI}(C_4 \vee K_{n-4}) > \text{AZI}(\overline{S_4} \vee K_{n-4}) > \text{AZI}(G).$$

Proof By direct computation, for $n \geq 5$, we have

$$\begin{aligned} \text{AZI}(\overline{S_3} \vee K_{n-3}) &= \frac{(n-3)(n-4)(n-1)^6}{2(2n-4)^3} + \frac{2(n-3)(n-1)^3(n-2)^3}{(2n-5)^3} + \\ &\quad \frac{(n-2)^6 + (n-3)^4(n-1)^3}{(2n-6)^3}, \end{aligned}$$

$$\begin{aligned}
 \text{AZI}(C_4 \vee K_{n-4}) &= \frac{(n-4)(n-5)(n-1)^6}{2(2n-4)^3} + \frac{4(n-4)(n-1)^3(n-2)^3}{(2n-5)^3} + \frac{4(n-2)^6}{(2n-6)^3}, \\
 \text{AZI}(\overline{S_4} \vee K_{n-4}) &= \frac{(n-4)(n-5)(n-1)^6}{2(2n-4)^3} + \frac{3(n-4)(n-1)^3(n-2)^3}{(2n-5)^3} + \\
 &\quad \frac{3(n-2)^6}{(2n-6)^3} + \frac{(n-1)^3(n-4)^4}{(2n-7)^3}, \\
 \text{AZI}(\overline{K_3} \vee K_{n-3}) &= \frac{(n-3)(n-4)(n-1)^6}{2(2n-4)^3} + \frac{3(n-1)^3(n-3)^4}{(2n-6)^3}, \\
 \text{AZI}(P_4 \vee K_{n-4}) &= \frac{(n-4)(n-5)(n-1)^6}{2(2n-4)^3} + \frac{2(n-4)(n-1)^3(n-2)^3}{(2n-5)^3} + \\
 &\quad \frac{2(n-4)(n-1)^3(n-3)^3 + (n-2)^6}{(2n-6)^3} + \frac{2(n-2)^3(n-3)^3}{(2n-7)^3}, \\
 \text{AZI}(\overline{S_3} \vee (K_{n-3} - e)) &= \frac{(n-5)(n-6)(n-1)^6}{2(2n-4)^3} + \frac{4(n-5)(n-1)^3(n-2)^3}{(2n-5)^3} + \\
 &\quad \frac{(n-5)(n-1)^3(n-3)^3 + 5(n-2)^6}{(2n-6)^3} + \frac{2(n-2)^3(n-3)^3}{(2n-7)^3}, \\
 \text{AZI}(C_4 \vee (K_{n-4} - e))(n \geq 6) &= \frac{(n-6)(n-7)(n-1)^6}{2(2n-4)^3} + \frac{12(n-2)^6}{(2n-6)^3} + \\
 &\quad \frac{6(n-6)(n-1)^3(n-2)^3}{(2n-5)^3}.
 \end{aligned}$$

It can be checked by calculator that for $n \geq 5$, $\text{AZI}(\overline{S_3} \vee K_{n-3}) - \text{AZI}(C_4 \vee K_{n-4}) > 0$, $\text{AZI}(C_4 \vee K_{n-4}) - \text{AZI}(\overline{S_4} \vee K_{n-4}) > 0$ and $\text{AZI}(\overline{S_4} \vee K_{n-4}) - \text{AZI}(G) > 0$, where $G \in \{\overline{K_3} \vee K_{n-3}, P_4 \vee K_{n-4}, \overline{S_3} \vee (K_{n-3} - e), C_4 \vee (K_{n-4} - e) \ (n \geq 6)\}$. \square

The following theorem gives the first five largest AZI indices of connected graphs with n vertices, where $n \geq 5$.

Theorem 2.4 *Let $G \in \mathbb{G}_n$ and $G \notin \{K_n, K_n - e, \overline{S_3} \vee K_{n-3}, C_4 \vee K_{n-4}, \overline{S_4} \vee K_{n-4}\}$, where $n \geq 5$. Then $\text{AZI}(K_n) > \text{AZI}(K_n - e) > \text{AZI}(\overline{S_3} \vee K_{n-3}) > \text{AZI}(C_4 \vee K_{n-4}) > \text{AZI}(\overline{S_4} \vee K_{n-4}) > \text{AZI}(G)$.*

Proof Since $G \in \mathbb{G}_n$ ($n \geq 5$) and $G \notin \{K_n, K_n - e, \overline{S_3} \vee K_{n-3}, C_4 \vee K_{n-4}, \overline{S_4} \vee K_{n-4}\}$, we have $G \in \cup_{n-1 \leq m \leq \binom{n}{2}-3} \mathbb{G}_{n,m}$. If $G \in \cup_{n-1 \leq m \leq \binom{n}{2}-4} \mathbb{G}_{n,m}$, then by Corollary 2.2, there exists a graph $G^* \in \mathbb{G}_{n, \binom{n}{2}-3}$ such that $\text{AZI}(G) < \text{AZI}(G^*)$. It follows from Lemma 2.3 that

$$\text{AZI}(G) < \text{AZI}(G^*) \leq \text{AZI}(\overline{S_4} \vee K_{n-4}). \tag{2.1}$$

If $G \in \mathbb{G}_{n, \binom{n}{2}-3}$, since $G \not\cong \overline{S_4} \vee K_{n-4}$, then we also have

$$\text{AZI}(G) < \text{AZI}(\overline{S_4} \vee K_{n-4}) \tag{2.2}$$

by Lemma 2.3. Moreover, $K_n \cong (K_n - e) + e$ and $K_n - e \cong (\overline{S_3} \vee K_{n-3}) + e$, then by Lemma 2.1, we obtain that

$$\text{AZI}(K_n) > \text{AZI}(K_n - e) > \text{AZI}(\overline{S_3} \vee K_{n-3}). \tag{2.3}$$

Combining inequalities (2.1)–(2.3) with the inequality

$$\text{AZI}(\overline{S_3} \vee K_{n-3}) > \text{AZI}(C_4 \vee K_{n-4}) > \text{AZI}(\overline{S_4} \vee K_{n-4})$$

in Lemma 2.3, we obtain the desired results. \square

3. Ordering trees by the AZI indices

Let x_{ij} be the number of edges of a graph G connecting vertices of degrees i and j , and let $A_{ij} = (\frac{ij}{i+j-2})^3$, where i, j are positive integers. Obviously, $x_{ij} = x_{ji}$ and $A_{ij} = A_{ji}$. Then the augmented Zagreb index of a graph G can be rewritten as $\text{AZI}(G) = \sum_{i \leq j} x_{ij} A_{ij}$.

Lemma 3.1 (1) A_{1j} is decreasing for $j \geq 2$.

(2) $A_{2j} = 8$ for $j \geq 1$.

(3) If $i (\geq 3)$ is fixed, then A_{ij} is increasing for $j \geq 2$.

Proof Clearly, $A_{2j} = (\frac{2j}{2+j-2})^3 = 8$ for $j \geq 1$. Note that

$$\frac{\partial(A_{ij})}{\partial j} = \frac{3i^3 j^2(i-2)}{(i+j-2)^4}.$$

Hence A_{1j} is decreasing and A_{ij} is increasing for $j \geq 2$, where $i (\geq 3)$ is fixed. \square

Let \mathbb{T}_n be the set of trees of order $n \geq 3$, and let $\mathbb{T}_{n,p}$ be the set of trees with n vertices and p pendent vertices, where $2 \leq p \leq n-1$. Then $\mathbb{T}_n = \cup_{2 \leq p \leq n-1} \mathbb{T}_{n,p}$. Let $DS_n(p_1, p_2)$ be the tree of order n formed from the path of order $n - p_1 - p_2$ by attaching p_1 and p_2 pendent vertices to its end vertices respectively, where $p_2 \geq p_1 \geq 1$ and $p_1 + p_2 \leq n - 2$. Clearly, $\mathbb{T}_{n,n-1} = \{S_n\}$, $\mathbb{T}_{n,n-2} = \{DS_n(p_1, n - 2 - p_1) | 1 \leq p_1 \leq \lfloor \frac{n-2}{2} \rfloor\}$ and $\mathbb{T}_{n,2} = \{DS_n(1, 1)\} = \{P_n\}$.

Theorem 3.2 Let $T \in \mathbb{T}_{n,p}$, where $2 \leq p \leq n - 3$. Then

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

with equality if and only if $T \cong DS_n(\lfloor \frac{p}{2} \rfloor, \lceil \frac{p}{2} \rceil)$.

Proof The case of $p = 2$ is trivial since $\mathbb{T}_{n,2} = \{DS_n(1, 1)\} = \{P_n\}$. Notice that there are t vertices, denoted by v_1, v_2, \dots, v_t , such that $\cup_{i=1}^t N(v_i)$ contains all pendent vertices of T . Suppose that there are p_i pendent vertices in $N(v_i)$, where $i = 1, 2, \dots, t$ and $\sum_{i=1}^t p_i = p$. Without loss of generality, we may assume that $p_i \geq 1$ for $1 \leq i \leq t$. Since $p \neq n - 1$ (namely, T is not a star), then $t \geq 2$. Hence

$$\text{AZI}(T) = \sum_{i=1}^t p_i A_{1,d_{v_i}} + \sum_{2 \leq i < j \leq n-1} x_{ij} A_{ij}. \tag{3.1}$$

Note that the terminal vertices of a diameter-achieving path P of T are two pendent vertices. Without loss of generality, suppose that the neighbors of the terminal vertices are v_1 and v_2 , respectively. By the choice of the diameter-achieving path P , we have $d_{v_1} = p_1 + 1$ and $d_{v_2} =$

$p_2 + 1$. Note that $d_{v_i} \geq 2$ for $1 \leq i \leq t$ and

$$\sum_{i=1}^t d_{v_i} \leq 2(n-1) - p - 2(n-p-t) = p + 2t - 2.$$

We claim that $d_{v_i} \leq p + 2 - d_{v_1}$ for $2 \leq i \leq t$. Otherwise, if $d_{v_i} > p + 2 - d_{v_1}$ for some $i \neq 1$, then

$$p + 2t - 2 \geq \sum_{i=1}^t d_{v_i} > d_{v_1} + (p + 2 - d_{v_1}) + 2(t-2) = p + 2t - 2,$$

which is a contradiction. Therefore, by Lemma 3.1, we have

$$\begin{aligned} \sum_{i=1}^t p_i A_{1,d_{v_i}} &= p_1 A_{1,d_{v_1}} + \sum_{i=2}^t p_i A_{1,d_{v_i}} \geq p_1 A_{1,d_{v_1}} + \sum_{i=2}^t p_i A_{1,p+2-d_{v_1}} \\ &= p_1 A_{1,p_1+1} + (p-p_1) A_{1,p-p_1+1}. \end{aligned}$$

If $\sum_{i=1}^t p_i A_{1,d_{v_i}} = p_1 A_{1,p_1+1} + (p-p_1) A_{1,p-p_1+1}$ and $t \geq 3$, then we get

$$p + 2t - 2 \geq \sum_{i=1}^t d_{v_i} \geq d_{v_1} + 2(p + 2 - d_{v_1}) + 2(t-3) = (p + 2t - 2) + (p - d_{v_1}),$$

equivalently, $d_{v_1} = p_1 + 1 \geq p$, which is a contradiction. Consequently, we conclude that

$$\sum_{i=1}^t p_i A_{1,d_{v_i}} \geq p_1 A_{1,p_1+1} + (p-p_1) A_{1,p-p_1+1} = \frac{(p_1+1)^3}{p_1^2} + \frac{(p-p_1+1)^3}{(p-p_1)^2}$$

with equality if and only if $t = 2$ and $d_{v_2} = p + 2 - d_{v_1} = p - p_1 + 1$, namely, $p_1 + p_2 = p$. Moreover, the function $f(x) = \frac{(x+1)^3}{x^2}$ is convex increasing for $x \geq 2$, since

$$f'(x) = \frac{(x+1)^2(x-2)}{x^3} \geq 0 \text{ and } f''(x) = \frac{6(x+1)}{x^4} > 0.$$

Besides, $f(1) = 8 > f(2) = \frac{27}{4}$, and then

$$f(1) + f(p-1) > f(2) + f(p-2) \geq \dots \geq f(\lfloor \frac{p}{2} \rfloor) + f(\lceil \frac{p}{2} \rceil).$$

It leads to

$$\sum_{i=1}^t p_i A_{1,d_{v_i}} \geq \frac{(p_1+1)^3}{p_1^2} + \frac{(p-p_1+1)^3}{(p-p_1)^2} \geq \frac{(\lfloor \frac{p}{2} \rfloor + 1)^3}{\lfloor \frac{p}{2} \rfloor^2} + \frac{(\lceil \frac{p}{2} \rceil + 1)^3}{\lceil \frac{p}{2} \rceil^2}.$$

The equality holds if and only if $t = 2$, $p_1 = \lfloor \frac{p}{2} \rfloor$ and $p_2 = \lceil \frac{p}{2} \rceil$.

On the other hand, it follows from Lemma 3.1 that

$$\sum_{2 \leq i \leq j \leq n-1} x_{ij} A_{ij} \geq \sum_{2 \leq i \leq j \leq n-1} x_{ij} A_{2j} = 8(n-1-p)$$

with equality holding if and only if all edges of T are pendent edges or the edges with one end vertex of degree 2.

All in all, it follows from Equation (3.1) that

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

with equality if and only if $T \cong DS_n(\lfloor \frac{p}{2} \rfloor, \lceil \frac{p}{2} \rceil)$. This completes the proof. \square

Corollary 3.3 *Let $T \in \cup_{2 \leq p \leq n-3} \mathbb{T}_{n,p}$. Then*

$$\text{AZI}(T) \geq \frac{(\lfloor \frac{n-3}{2} \rfloor + 1)^3}{\lfloor \frac{n-3}{2} \rfloor^2} + \frac{(\lceil \frac{n-3}{2} \rceil + 1)^3}{\lceil \frac{n-3}{2} \rceil^2} + 16$$

with equality if and only if $T \cong DS_n(\lfloor \frac{n-3}{2} \rfloor, \lceil \frac{n-3}{2} \rceil)$.

Proof By Theorem 3.2, it will suffice to show that $\text{AZI}(DS_n(\lfloor \frac{p-1}{2} \rfloor, \lceil \frac{p-1}{2} \rceil)) > \text{AZI}(DS_n(\lfloor \frac{p}{2} \rfloor, \lceil \frac{p}{2} \rceil))$, where $3 \leq p \leq n-3$. By Lemma 3.1, we have

$$\begin{aligned} \text{AZI}(DS_n(\lfloor \frac{p}{2} \rfloor, \lceil \frac{p}{2} \rceil)) &= \lfloor \frac{p}{2} \rfloor A_{1, \lfloor \frac{p}{2} \rfloor + 1} + \lceil \frac{p}{2} \rceil A_{1, \lceil \frac{p}{2} \rceil + 1} + 8(n-1-p) \\ &= \lceil \frac{p-1}{2} \rceil A_{1, \lceil \frac{p-1}{2} \rceil + 1} + \lfloor \frac{p-1}{2} \rfloor A_{1, \lfloor \frac{p-1}{2} \rfloor + 1} + A_{1, \lceil \frac{p}{2} \rceil + 1} + 8(n-1-p) \\ &< \lceil \frac{p-1}{2} \rceil A_{1, \lceil \frac{p-1}{2} \rceil + 1} + \lfloor \frac{p-1}{2} \rfloor A_{1, \lfloor \frac{p-1}{2} \rfloor + 1} + 8 + 8(n-1-p) \\ &= \text{AZI}(DS_n(\lfloor \frac{p-1}{2} \rfloor, \lceil \frac{p-1}{2} \rceil)). \quad \square \end{aligned}$$

An order of trees in $\mathbb{T}_{n,n-2}$ ($n \geq 4$) by their AZI indices is given as follows.

Lemma 3.4 *Observe that $\mathbb{T}_{n,n-2} = \{DS_n(p_1, n-2-p_1) | 1 \leq p_1 \leq \lfloor \frac{n-2}{2} \rfloor\}$. Then*

$$\text{AZI}(DS_n(\lfloor \frac{n-2}{2} \rfloor, \lceil \frac{n-2}{2} \rceil)) > \dots > \text{AZI}(DS_n(2, n-4)) > \text{AZI}(DS_n(1, n-3)).$$

Proof For $1 \leq p_1 \leq \lfloor \frac{n-2}{2} \rfloor$, note that

$$\text{AZI}(DS_n(p_1, n-2-p_1)) = \frac{(p_1+1)^3}{p_1^2} + \frac{(n-1-p_1)^3}{(n-2-p_1)^2} + \frac{(p_1+1)^3(n-1-p_1)^3}{(n-2)^3} := f(p_1).$$

The result follows since the function $f(p_1)$ is increasing for $1 \leq p_1 \leq \lfloor \frac{n-2}{2} \rfloor$. \square

Let $T_6^*, T_7^*, T_7^{**}, T_7^{***}$ be the trees as shown in Figure 1.



Figure 1 $T_6^*, T_7^*, T_7^{**}, T_7^{***}$

Now we obtain an order of \mathbb{T}_n for $3 \leq n \leq 7$ by their AZI indices. Observe that $\mathbb{T}_3 = \{S_3\}$, $\mathbb{T}_4 = \{P_4, S_4\}$, $\mathbb{T}_5 = \{P_5, DS_5(1, 2), S_5\}$,

$$\text{AZI}(P_4) > \text{AZI}(S_4) \quad \text{and} \quad \text{AZI}(P_5) > \text{AZI}(DS_5(1, 2)) > \text{AZI}(S_5). \quad (3.2)$$

Note that $\mathbb{T}_6 = \{P_6, T_6^*, DS_6(1, 2), DS_6(2, 2), DS_6(1, 3), S_6\}$,

$$\begin{aligned} \text{AZI}(P_6) &> \text{AZI}(T_6^*) > \text{AZI}(DS_6(1, 2)) \\ &> \text{AZI}(DS_6(2, 2)) > \text{AZI}(DS_6(1, 3)) > \text{AZI}(S_6), \end{aligned} \quad (3.3)$$

and $\mathbb{T}_7 = \{P_7, T_7^*, DS_7(1, 2), T_7^{**}, T_7^{***}, DS_7(1, 3), DS_7(2, 2), DS_7(2, 3), DS_7(1, 4), S_7\}$,

$$\text{AZI}(P_7) > \text{AZI}(T_7^*) > \text{AZI}(DS_7(1, 2)) > \text{AZI}(T_7^{**})$$

$$\begin{aligned} &> \text{AZI}(T_7^{***}) > \text{AZI}(DS_7(1, 3)) > \text{AZI}(DS_7(2, 2)) \\ &> \text{AZI}(DS_7(2, 3)) > \text{AZI}(DS_7(1, 4)) > \text{AZI}(S_7). \end{aligned} \tag{3.4}$$

Moreover, the trees of order $n \geq 8$ with the first three smallest AZI indices are determined.

Theorem 3.5 *Let $T \in \mathbb{T}_n$ and $T \not\cong S_n, DS_n(1, n-3), DS_n(\lfloor \frac{n-3}{2} \rfloor, \lceil \frac{n-3}{2} \rceil)$, where $n \geq 8$. Then $\text{AZI}(S_n) < \text{AZI}(DS_n(1, n-3)) < \text{AZI}(DS_n(\lfloor \frac{n-3}{2} \rfloor, \lceil \frac{n-3}{2} \rceil)) < \text{AZI}(T)$.*

Proof It is obvious that

$$\begin{aligned} \text{AZI}(S_n) &= (n-3)A_{1,n-1} + 2A_{1,n-1} < (n-3)A_{1,n-2} + 16 = \text{AZI}(DS_n(1, n-3)) \\ &< \lceil \frac{n-3}{2} \rceil A_{1, \lceil \frac{n-3}{2} \rceil + 1} + \lfloor \frac{n-3}{2} \rfloor A_{1, \lfloor \frac{n-3}{2} \rfloor + 1} + 16 \\ &= \text{AZI}(DS_n(\lfloor \frac{n-3}{2} \rfloor, \lceil \frac{n-3}{2} \rceil)). \end{aligned}$$

Since $T \in \mathbb{T}_n$ ($n \geq 8$) and $T \not\cong S_n, DS_n(1, n-3), DS_n(\lfloor \frac{n-3}{2} \rfloor, \lceil \frac{n-3}{2} \rceil)$, we consider the following two cases.

Case 1 $T \in \mathbb{T}_{n,n-2} = \{DS_n(p_1, n-2-p_1) | 1 \leq p_1 \leq \lfloor \frac{n-2}{2} \rfloor\}$. By Lemma 3.4, we need to prove that $\text{AZI}(DS_n(2, n-4)) > \text{AZI}(DS_n(\lfloor \frac{n-3}{2} \rfloor, \lceil \frac{n-3}{2} \rceil))$ for $n \geq 8$. By Theorem 3.2,

$$\begin{aligned} \text{AZI}(DS_n(\lfloor \frac{n-3}{2} \rfloor, \lceil \frac{n-3}{2} \rceil)) &< \text{AZI}(DS_n(2, n-5)) \\ &= 2A_{1,3} + 16 + (n-5)A_{1,n-4} \\ &< 2A_{1,3} + A_{3,n-3} + (n-4)A_{1,n-3} \\ &= \text{AZI}(DS_n(2, n-4)). \end{aligned}$$

Case 2 $T \in \cup_{2 \leq p \leq n-3} \mathbb{T}_{n,p}$. By Corollary 3.3, we immediately get

$$\text{AZI}(DS_n(\lfloor \frac{n-3}{2} \rfloor, \lceil \frac{n-3}{2} \rceil)) < \text{AZI}(T). \quad \square$$

By using Theorem 3.5, we obtain the first two smallest AZI indices of connected graphs with $n \geq 5$ vertices as follows.

Theorem 3.6 *Let $G \in \mathbb{G}_n$ and $G \not\cong S_n, DS_n(1, n-3)$, where $n \geq 5$. Then*

$$\text{AZI}(S_n) < \text{AZI}(DS_n(1, n-3)) < \text{AZI}(G).$$

Proof From inequalities (3.2)–(3.4) and Theorem 3.5, the inequality $\text{AZI}(S_n) < \text{AZI}(DS_n(1, n-3))$ holds for $n \geq 5$. Note that $G \in \cup_{n-1 \leq m \leq \binom{n}{2}} \mathbb{G}_{n,m}$. We have the following two cases.

Case 1 $G \in \mathbb{G}_{n,n-1} = \mathbb{T}_n$ ($n \geq 5$). By inequalities (3.2)–(3.4) and Theorem 3.5,

$$\text{AZI}(DS_n(1, n-3)) < \text{AZI}(G).$$

Case 2 $G \in \cup_{n \leq m \leq \binom{n}{2}} \mathbb{G}_{n,m}$. By Corollary 2.2, there exists a graph $G^* \in \mathbb{G}_{n,n-1}$ such that $\text{AZI}(G^*) < \text{AZI}(G)$. If $G^* \not\cong S_n$, then we immediately get $\text{AZI}(DS_n(1, n-3)) \leq \text{AZI}(G^*) < \text{AZI}(G)$. If $G^* \cong S_n$, then by Lemma 2.1, we conclude that G is obtained from S_n by inserting

some edges. It follows that

$$\begin{aligned} \text{AZI}(G) &\geq \text{AZI}(S_n^+) = 24 + (n-3)A_{1,n-1} \\ &> 16 + (n-3)A_{1,n-2} = \text{AZI}(DS_n(1, n-3)). \quad \square \end{aligned}$$

4. Unicyclic graphs with the first two smallest AZI indices

Denote by $C_{n,p}$ the unicyclic graph of order n formed by attaching p pendent vertices to a vertex of the cycle C_{n-p} , where $0 \leq p \leq n-3$. Let $C_{n,p}^{p_1, p_2, \dots, p_{n-p}}$ denote the unicyclic graph of order n obtained from the cycle $C_{n-p} = v_1 v_2 \cdots v_{n-p} v_1$ by attaching p_i pendent vertices to vertex v_i , where $p_i \geq 0$, $i = 1, 2, \dots, n-p$ and $\sum_{i=1}^{n-p} p_i = p$. Clearly, $C_{n,0} \cong C_n$, $C_{n,n-3} \cong S_n^+$ and $C_{n,p}^{p,0,\dots,0} \cong C_{n,p}$.

Let U_5^* be the unicyclic graph obtained by identifying one vertex of C_3 and one end vertex of P_3 . Let \mathbb{U}_n be the set of unicyclic graphs of order $n \geq 3$. Obviously, $\mathbb{U}_3 = \{K_3\}$, $\mathbb{U}_4 = \{C_4, S_4^+\}$ and $\mathbb{U}_5 = \{C_5, S_5^+, C_{5,1}, C_{5,2}^{1,1,0}, U_5^*\}$. By simply calculating, we get that $\text{AZI}(S_4^+) < \text{AZI}(C_4)$ and $\text{AZI}(S_5^+) < \text{AZI}(C_{5,2}^{1,1,0}) < \text{AZI}(C_{5,1}) < \text{AZI}(C_5) = \text{AZI}(U_5^*)$.

Let $\mathbb{U}_{n,p}$ be the set of unicyclic graphs with n vertices and p pendent vertices, where $0 \leq p \leq n-3$. Then $\mathbb{U}_n = \cup_{0 \leq p \leq n-3} \mathbb{U}_{n,p}$.

Lemma 4.1 ([5]) *Let $U \in \mathbb{U}_{n,p}$, where $0 \leq p \leq n-3$. Then*

$$\text{AZI}(U) \geq \frac{p(p+2)^3}{(p+1)^3} + 8(n-p)$$

with equality if and only if $U \cong C_{n,p}$.

Lemma 4.2 *Let $C_{n,p}$ be the unicyclic graph of order n defined above, where $0 \leq p \leq n-3$. Then $\text{AZI}(C_{n,0}) > \text{AZI}(C_{n,1}) > \cdots > \text{AZI}(C_{n,n-4}) > \text{AZI}(C_{n,n-3})$.*

Proof Note that $\text{AZI}(C_{n,p}) = \frac{p(p+2)^3}{(p+1)^3} + 8(n-p)$. Let $f(x) = \frac{x(x+2)^3}{(x+1)^3} + 8(n-x)$. Then

$$f'(x) = -\frac{x(7x^3 + 28x^2 + 42x + 24)}{(x+1)^4} \leq 0.$$

Thus $f(x)$ is decreasing for $x \geq 0$. This completes the proof. \square

By Lemmas 4.1 and 4.2, it is easy to obtain the following corollary.

Corollary 4.3 *Let $U \in \cup_{0 \leq p \leq n-4} \mathbb{U}_{n,p}$. Then*

$$\text{AZI}(U) \geq \frac{(n-4)(n-2)^3}{(n-3)^3} + 32$$

with equality if and only if $U \cong C_{n,n-4}$.

Lemma 4.4 *Let $U \in \mathbb{U}_{n,n-3}$ and $U \not\cong S_n^+$, where $n \geq 6$. Then $\text{AZI}(U) > \text{AZI}(C_{n,n-4}) > \text{AZI}(S_n^+)$.*

Proof Since $U \in \mathbb{U}_{n,n-3}$, we may assume that $G \cong C_{n,n-3}^{p_1, p_2, p_3}$, where $p_1 \geq p_2 \geq p_3 \geq 0$ and $\sum_{i=1}^3 p_i = n-3$. Notice that $U \not\cong S_n^+$, then $p_2 \geq 1$. Let $r = (p_1 - 1)(A_{1,p_1+2} - A_{1,n-2}) +$

$$p_2(A_{1,p_2+2} - A_{1,n-2}) + p_3(A_{1,p_3+2} - A_{1,n-2}).$$

Case 1 $p_3 = 0$. Since $n \geq 6$, then $p_1 \geq 2$. By Lemma 3.1, we have $r > 0$ and

$$AZI(U) - AZI(C_{n,n-4}) = r + A_{1,p_1+2} + A_{p_1+2,p_2+2} - 16. \quad (4.1)$$

Subcase 1.1 $p_1 = 2$. It follows from (4.1) and Lemma 3.1 that

$$AZI(U) - AZI(C_{n,n-4}) > 0 + A_{1,4} + A_{4,3} - 16 = \frac{4^3}{3^3} + \frac{12^3}{5^3} - 16 > 0.$$

Subcase 1.2 $p_1 \geq 3$. Then by Lemma 3.1 and (4.1), we have

$$AZI(U) - AZI(C_{n,n-4}) > 0 + 1 + A_{5,3} - 16 = 1 + \frac{15^3}{6^3} - 16 > 0.$$

Case 2 $p_3 \geq 1$. By Lemma 3.1, we obtain that $r > 0$ and

$$\begin{aligned} AZI(U) - AZI(C_{n,n-4}) &= r + A_{1,p_1+2} + A_{p_1+2,p_2+2} + A_{p_1+2,p_3+2} + A_{p_2+2,p_3+2} - 32 \\ &> 0 + 1 + 3A_{3,3} - 32 = 1 + 3 \cdot \frac{9^3}{4^3} - 32 > 0. \end{aligned}$$

Combining the above cases, we get that $AZI(U) > AZI(C_{n,n-4})$. Moreover, it is easy to obtain that $AZI(C_{n,n-4}) = (n-4)A_{1,n-2} + 32 > AZI(S_n^+) = (n-3)A_{1,n-1} + 24$. \square

It follows from Corollary 4.3 and Lemma 4.4 that the unicyclic graphs of order $n \geq 6$ with the minimum and the second minimum AZI indices are determined.

Theorem 4.5 *Let $U \in \mathbb{U}_n$ and $G \not\cong S_n^+, C_{n,n-4}$, where $n \geq 6$. Then*

$$AZI(S_n^+) < AZI(C_{n,n-4}) < AZI(U).$$

5. Bicyclic graphs with the minimum AZI index

Let \mathbb{B}_n be the set of bicyclic graphs of order $n \geq 4$. Clearly, $\mathbb{B}_4 = \{K_4 - e\}$. Let $\mathbb{B}_{n,p}$ be the set of bicyclic graphs with n vertices and p pendent vertices, where $0 \leq p \leq n-4$. Then $\mathbb{B}_n = \cup_{0 \leq p \leq n-4} \mathbb{B}_{n,p}$.

Denote by $D_{n,r,s,p}$ the bicyclic graph of order n by identifying one vertex of two cycles C_r and C_s , and attaching p pendent vertices to the common vertex, where $r \geq s \geq 3$ and $0 \leq p = n+1-r-s \leq n-5$.

Lemma 5.1 ([5]) *Let $B \in \mathbb{B}_{n,p}$, where $0 \leq p \leq n-5$. Then*

$$AZI(B) \geq \frac{p(p+4)^3}{(p+3)^3} + 8(n+1-p)$$

with equality if and only if $B \cong D_{n,r,s,p}$, where $r \geq s \geq 3$ and $r+s = n+1-p$.

Lemma 5.2 *Let $D_{n,r,s,p}$ be the bicyclic graph of order n defined above, where $r \geq s \geq 3$ and $0 \leq p = n+1-r-s \leq n-5$. Then $AZI(D_{n,r,s,0}) > AZI(D_{n,r,s,1}) > \dots > AZI(D_{n,r,s,n-5})$.*

Proof Observe that

$$AZI(D_{n,r,s,p}) = \frac{p(p+4)^3}{(p+3)^3} + 8(n+1-p) := g(p).$$

Then

$$g'(p) = -\frac{7p^4 + 84p^3 + 372p^2 + 704p + 456}{(p+3)^4} < 0.$$

Hence $g(p)$ is decreasing for $p \geq 0$. The proof is completed. \square

It can be seen from Lemmas 5.1 and 5.2 that

Corollary 5.3 *Let $B \in \cup_{0 \leq p \leq n-5} \mathbb{B}_{n,p}$. Then $\text{AZI}(B) \geq \frac{(n-5)(n-1)^3}{(n-2)^3} + 48$ with equality if and only if $B \cong D_{n,3,3,n-5}$.*

Now we consider the set $\mathbb{B}_{n,n-4}$, where $n \geq 5$. Let $E_n^{p_1,p_2,p_3,p_4}$ be the bicyclic graph obtained from $K_4 - e$ by attaching p_i pendent vertices to vertex $v_i \in V(K_4 - e)$ for $1 \leq i \leq 4$, where $d_{v_1} = d_{v_2} = 3$, $d_{v_3} = d_{v_4} = 2$, $p_1 \geq p_2 \geq 0$, $p_3 \geq p_4 \geq 0$ and $\sum_{i=1}^4 p_i = n - 4$. Then $\mathbb{B}_{n,n-4} = \{E_n^{p_1,p_2,p_3,p_4} | p_1 \geq p_2 \geq 0, p_3 \geq p_4 \geq 0 \text{ and } \sum_{i=1}^4 p_i = n - 4\}$.

Lemma 5.4 *Let $B \in \mathbb{B}_{n,n-4}$, where $n \geq 5$. Then*

$$\text{AZI}(B) \geq \frac{(n-4)(n-1)^3}{(n-2)^3} + \frac{27(n-1)^3}{n^3} + 32$$

with equality if and only if $B \cong E_n^{n-4,0,0,0}$.

Proof Let $B \cong E_n^{p_1,p_2,p_3,p_4}$, where $p_1 \geq p_2 \geq 0, p_3 \geq p_4 \geq 0$ and $\sum_{i=1}^4 p_i = n - 4$. Note that

$$\begin{aligned} \text{AZI}(E_n^{p_1,p_2,p_3,p_4}) &= p_1 A_{1,p_1+3} + p_2 A_{1,p_2+3} + p_3 A_{1,p_3+2} + \\ &\quad p_4 A_{1,p_4+2} + A_{p_1+3,p_2+3} + A_{p_1+3,p_3+2} + \\ &\quad A_{p_1+3,p_4+2} + A_{p_2+3,p_3+2} + A_{p_2+3,p_4+2}. \end{aligned}$$

Let $r = p_1(A_{1,p_1+3} - A_{1,n-1}) + p_2(A_{1,p_2+3} - A_{1,n-1}) + p_3(A_{1,p_3+2} - A_{1,n-1}) + p_4(A_{1,p_4+2} - A_{1,n-1})$. Then by Lemma 3.1, we have $r \geq 0$ with equality holding if and only if $p_1 = n - 4$ and $p_2 = p_3 = p_4 = 0$. Now we discuss the following cases.

Case 1 $p_2 \geq 1$. Then $p_1 \geq p_2 \geq 1$.

Subcase 1.1 $p_3 \geq 1$. It follows from Lemma 3.1 that

$$\begin{aligned} \text{AZI}(B) - \text{AZI}(E_n^{n-4,0,0,0}) &= r + A_{p_1+3,p_2+3} + A_{p_1+3,p_3+2} + A_{p_1+3,p_4+2} + \\ &\quad A_{p_2+3,p_3+2} + A_{p_2+3,p_4+2} - A_{3,n-1} - 32 \\ &> 0 + A_{4,4} + 2A_{4,3} + 2A_{4,2} - A_{3,n-1} - 32 \\ &> 0 + \frac{16^3}{6^3} + 2 \cdot \frac{12^3}{5^3} + 16 - 27 - 32 > 0. \end{aligned}$$

Subcase 1.2 $p_3 = 0$. Then $p_4 = 0$. Hence by Lemma 3.1, we have

$$\begin{aligned} \text{AZI}(B) - \text{AZI}(E_n^{n-4,0,0,0}) &= r + A_{p_1+3,p_2+3} - A_{3,n-1} \\ &> 0 + \frac{[p_1 p_2 + 3(n-1)]^3 - [3(n-1)]^3}{n^3} > 0. \end{aligned}$$

Case 2 $p_2 = 0$. Let $q(x) = A_{3,x}$. Then $q(x)$ is concave increasing for $x \geq 2$ since

$$q'(x) = \frac{81x^2}{(x+1)^4} > 0 \text{ and } q''(x) = -\frac{162x(x-1)}{(x+1)^5} < 0.$$

It follows that

$$A_{3, \lceil \frac{n}{2} \rceil} + A_{3, \lfloor \frac{n}{2} \rfloor} > \cdots > A_{3, n-2} + A_{3, 2}, \quad (5.1)$$

$$A_{3, \lceil \frac{n+1}{2} \rceil} + A_{3, \lfloor \frac{n+1}{2} \rfloor} > \cdots > A_{3, n-1} + A_{3, 2}. \quad (5.2)$$

Subcase 2.1 $p_4 \geq 1$. Then $p_3 \geq p_4 \geq 1$. If $p_1 \geq 1$, then by Lemma 3.1,

$$\begin{aligned} \text{AZI}(B) - \text{AZI}(E_n^{n-4, 0, 0, 0}) &\geq r + 3A_{4, 3} + 2A_{3, 3} - A_{3, n-1} - 32 \\ &> 0 + 3 \cdot \frac{12^3}{5^3} + 2 \cdot \frac{9^3}{4^3} - 27 - 32 > 0. \end{aligned}$$

If $p_1 = 0$, then by Lemma 3.1 and the inequality (5.1), for $n \geq 5$ we have

$$\begin{aligned} \text{AZI}(B) - \text{AZI}(E_n^{n-4, 0, 0, 0}) &= r + A_{3, 3} + 2(A_{3, p_3+2} + A_{3, p_4+2}) - A_{3, n-1} - 32 \\ &> 0 + A_{3, 3} + 2(A_{3, n-2} + A_{3, 2}) - A_{3, n-1} - 32 \\ &= \frac{(n-4)(1433n^5 - 3751n^4 - 337n^3 + 5859n^2 - 2484n + 432)}{64n^3(n-1)^3} > 0. \end{aligned}$$

Subcase 2.2 $p_4 = 0$. It follows from Lemma 3.1 and the inequality (5.2) that

$$\begin{aligned} \text{AZI}(B) - \text{AZI}(E_n^{n-4, 0, 0, 0}) &= r + (A_{3, p_1+3} + A_{3, p_3+2}) + A_{p_1+3, p_3+2} - A_{3, n-1} - 16 \\ &\geq 0 + (A_{3, n-1} + A_{3, 2}) + A_{p_1+3, p_3+2} - A_{3, n-1} - 16 \\ &= A_{p_1+3, p_3+2} - 8 \geq 0 \end{aligned}$$

with equality if and only if $p_1 = n - 4$ and $p_2 = p_3 = p_4 = 0$, that is, $B \cong E_n^{n-4, 0, 0, 0}$. \square

The bicyclic graph of order $n \geq 5$ with the minimum AZI index is characterized in the following theorem.

Theorem 5.5 Let $B \in \mathbb{B}_n$ and $B \not\cong D_{n, 3, 3, n-5}$, where $n \geq 5$. Then $\text{AZI}(D_{n, 3, 3, n-5}) < \text{AZI}(B)$.

Proof Note that $\mathbb{B}_n = \cup_{0 \leq p \leq n-4} \mathbb{B}_{n, p}$. Then by Corollary 5.3 and Lemma 5.4, it will suffice to prove that for $n \geq 5$, $\text{AZI}(D_{n, 3, 3, n-5}) < \text{AZI}(E_n^{n-4, 0, 0, 0})$. It is obvious that

$$\text{AZI}(E_n^{n-4, 0, 0, 0}) - \text{AZI}(D_{n, 3, 3, n-5}) = \frac{27(n-1)^3}{n^3} + \frac{(n-1)^3}{(n-2)^3} - 16 > 0.$$

This completes the proof of Theorem 5.5. \square

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