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

\[
AZI(G) = \sum_{u \neq v \in E(G)} \left( \frac{d_u d_v}{d_u + d_v - 2} \right)^3,
\]

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 QSAR/QSPR 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

\[
AZI(G) = \sum_{u \neq v \in E(G)} \left( \frac{d_u d_v}{d_u + d_v - 2} \right)^3.
\]

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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 \( G_1 \lor G_2 \) 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 \( G_n \) be the set of connected graphs of order \( n \), and let \( G_{n,m} \) be the set of connected graphs with \( n \) vertices and \( m \) edges, where \( n - 1 \leq m \leq \binom{n}{2} \). Obviously, \( G_1 = \{K_1\} \), \( G_2 = \{K_2\} \) and \( G_n = \bigcup_{1 \leq m \leq \binom{n}{2}} G_{n,m} \). Now we shall investigate the AZI index of \( G \in G_n \) for \( n \geq 3 \). To begin with, a key lemma to obtain our main results is given as follows.

**Lemma 2.1** ([5]) Let \( G \in G_n \) and \( G \nsubseteq K_n \), where \( n \geq 3 \). Then for \( e \notin E(G) \), \( AZI(G) < AZI(G + e) \).

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 \( G_1 \in G_{n,m_1} \). Then there exists a graph \( G_2 \in G_{n,m_2} \) such that \( AZI(G_2) > AZI(G_1) \).
2. Let \( G_2 \in G_{n,m_2} \). Then there exists a graph \( G_1 \in G_{n,m_1} \) such that \( AZI(G_1) < AZI(G_2) \).

Observe that \( G_3 = \{K_3, P_3\} \) and \( G_4 = \{K_4, K_4 - e, C_4, S^+_{4}, P_4, S_4\} \). By Corollary 2.2 and simply calculating, we immediately get \( AZI(K_3) > AZI(P_3) \) and

\[
AZI(K_4) > AZI(K_4 - e) > AZI(C_4) > AZI(S^+_4) > AZI(P_4) > AZI(S_4).
\]

For \( n \geq 5 \), observe that \( G_{n,\binom{n}{2}} - 3 \) is closed to \( \{K_n\} \), \( G_{n,\binom{n}{2}} - \{K_n - e\} \), \( G_{n,\binom{n}{2}} - 2 \) is closed to \( \{\overline{K}_n \lor K_{n-3}, C_4 \lor K_{n-4}\} \) and \( G_{n,\binom{n}{2}} - 3 \) is closed to \( \{\overline{S}_3 \lor P_4, \overline{K}_3 \lor P_4, \overline{K}_3 \lor S_4, \overline{K}_3 \lor (K_{n-3} - e), C_4 \lor (K_{n-4} - e) \} \).

**Lemma 2.3** Let \( G \in G_{n,\binom{n}{2}} - 3 \) and \( G \nsubseteq S_3 \lor K_{n-4} \). Then for \( n \geq 5 \),

\[
AZI(S_3 \lor K_{n-3}) > AZI(C_4 \lor K_{n-4}) > AZI(S_3 \lor K_{n-4}) > AZI(G).
\]

**Proof** By direct computation, for \( n \geq 5 \), we have

\[
AZI(S_3 \lor K_{n-3}) = \frac{(n - 3)(n - 4)(n - 1)^6}{2(2n - 4)^3} + \frac{2(n - 3)(n - 1)^3(n - 2)^3}{(2n - 5)^3} + \frac{(n - 2)^6 + (n - 3)^4(n - 1)^3}{(2n - 6)^3}.
\]
It can be checked by calculator that for $n \geq 5$, $\text{AZI}(\overline{3} \vee K_{n-3}) - \text{AZI}(C_4 \vee K_{n-4}) > 0$, $\text{AZI}(C_4 \vee K_{n-4}) - \text{AZI}(\overline{3} \vee K_{n-4}) > 0$ and $\text{AZI}(\overline{3} \vee K_{n-4}) - \text{AZI}(G) > 0$, where $G \in \{ \overline{3} \vee K_{n-3}, P_4 \vee K_{n-4}, \overline{3} \vee (K_{n-3} - e), C_4 \vee (K_{n-4} - e) \}$ ($n \geq 6$).

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 $G \notin \{ K_n, K_n - e, \overline{3} \vee K_{n-3}, C_4 \vee K_{n-4}, \overline{3} \vee K_{n-4} \}$, where $n \geq 5$. Then $\text{AZI}(K_n) > \text{AZI}(K_n - e) > \text{AZI}(\overline{3} \vee K_{n-3}) > \text{AZI}(C_4 \vee K_{n-4}) > \text{AZI}(\overline{3} \vee K_{n-4}) > \text{AZI}(G)$.

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

$$\text{AZI}(G) < \text{AZI}(G^*) \leq \text{AZI}(\overline{3} \vee K_{n-4}). \quad (2.1)$$

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

$$\text{AZI}(G) < \text{AZI}(\overline{3} \vee K_{n-4}) \quad (2.2)$$

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

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

Furthermore, $\text{AZI}(K_n - e) > \text{AZI}(\overline{3} \vee K_{n-4})$, so we have $\text{AZI}(K_n) > \text{AZI}(K_n - e) > \text{AZI}(\overline{3} \vee K_{n-3})$. 

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

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

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

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

Thus, $\text{AZI}(G) < \text{AZI}(G^*) \leq \text{AZI}(\overline{3} \vee K_{n-4})$.
Combining inequalities (2.1)–(2.3) with the inequality
\[ \text{AZI}(S_3 \vee K_{n-3}) > \text{AZI}(C_4 \vee K_{n-4}) > \text{AZI}(S_4 \vee K_{n-4}) \]
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. \(A_{ij}\) is decreasing for \(j \geq 2\).
2. \(A_{ij} = 8\) for \(j \geq 1\).
3. If \(i \geq 3\) is fixed, then \(A_{ij}\) is increasing for \(j \geq 2\).

**Proof**  
Clearly, \(A_{2j} = (\frac{2i}{2j-2})^3 = 8\) for \(j \geq 1\). Note that
\[ \frac{\partial(A_{ij})}{\partial j} = \frac{3i^2j^2(i-2)}{(i+j-2)^3} \]
Hence \(A_{ij}\) is decreasing and \(A_{ij}\) is increasing for \(j \geq 2\), where \(i \geq 3\) is fixed. \(\square\)

Let \(T_n\) be the set of trees of order \(n \geq 3\), and let \(T_{n,p}\) be the set of trees with \(n\) vertices and \(p\) pendant vertices, where \(2 \leq p \leq n-1\). Then \(T_n = \cup_{2 \leq p \leq n-1} T_{n,p}\). 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 \(p_2\) pendant vertices to its end vertices respectively, where \(p_2 \geq p_1 \geq 1\) and \(p_1 + p_2 \leq n-2\). Clearly, \(T_{n,n-2} = \{DS_n(p_1, n-2-p_1)| 1 \leq p_1 \leq \lfloor \frac{n-2}{2} \rfloor \}\) and \(T_{n,2} = \{DS_n(1,1)\}\).

**Theorem 3.2**  
Let \(T \in T_{n,p}\), where \(2 \leq p \leq n-3\). Then
\[ \text{AZI}(T) \geq \frac{(\lfloor \frac{n}{2} \rfloor + 1)^3}{(\lfloor \frac{n}{2} \rfloor)^2} + \frac{(\lceil \frac{n}{2} \rceil + 1)^3}{(\lceil \frac{n}{2} \rceil)^2} + 8(n-1-p) \]
with equality if and only if \(T \equiv DS_n(\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil)\).

**Proof**  
The case of \(p = 2\) is trivial since \(T_{n,2} = \{DS_n(1,1)\}\) = \(\{P_n\}\). Notice that there are \(t\) vertices, denoted by \(v_1, v_2, \ldots, v_t\), such that \(\cup_{i=1}^t N(v_i)\) contains all pendant vertices of \(T\). Suppose that there are \(p_i\) pendant vertices in \(N(v_i)\), where \(i = 1, 2, \ldots, t\) 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
\[ \text{AZI}(T) = \sum_{i=1}^t p_i A_{v_i} + \sum_{2 \leq i \leq n-1} x_{ij}A_{ij}. \]  
(3.1)

Note that the terminal vertices of a diameter-achieving path \(P\) of \(T\) are two pendant 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 \(d_{v_2} = \ldots\).
Moreover, the function $f$ vertex of degree 2.

We claim that $d_{vi} \leq p + 2 - d_{v1}$ for $2 \leq i \leq t$. Otherwise, if $d_{vi} > p + 2 - d_{v1}$ for some $i \neq 1$, then

$$p + 2t - 2 \geq \sum_{i=1}^{t} d_{vi} > d_{v1} + (p + 2 - d_{v1}) + 2(t - 2) = p + 2t - 2,$$

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

$$\sum_{i=1}^{t} p_{i} A_{1,d_{vi}} = p_{1} A_{1,d_{v1}} + \sum_{i=2}^{t} p_{i} A_{1,d_{vi}} \geq p_{1} A_{1,d_{v1}} + \sum_{i=2}^{t} p_{i} A_{1,p+2-d_{vi}} = p_{1} A_{1,p+1} + (p - p_{1}) A_{1,p-p_{1}+1}.$$ 

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

$$p + 2t - 2 \geq \sum_{i=1}^{t} d_{vi} \geq d_{v1} + 2(p + 2 - d_{v1}) + 2(t - 3) = (p + 2t - 2) + (p - d_{v1}),$$

equivalently, $d_{v1} = p_{1} + 1 \geq p$, which is a contradiction. Consequently, we conclude that

$$\sum_{i=1}^{t} p_{i} A_{1,d_{vi}} \geq p_{1} A_{1,p+1} + (p - p_{1}) A_{1,p-p_{1}+1} = \left(\frac{p_{1} + 1}{p_{1}^{2}}\right)^{3} + \frac{(p - p_{1} + 1)^{3}}{(p - p_{1})^{2}}$$

with equality if and only if $t = 2$ and $d_{v2} = p + 2 - d_{v1} = p - p_{1} + 1$, 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

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

It leads to

$$\sum_{i=1}^{t} p_{i} A_{1,d_{vi}} \geq \left(\frac{p_{1} + 1}{p_{1}^{2}}\right)^{3} + \frac{(p - p_{1} + 1)^{3}}{(p - p_{1})^{2}} \geq \left(\frac{\lfloor \frac{p}{2} \rfloor + 1}{\lfloor \frac{p}{2} \rfloor^{2}}\right)^{3} + \frac{(\lfloor \frac{p}{2} \rfloor + 1)^{3}}{(\lfloor \frac{p}{2} \rfloor)^{2}}.$$

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

$$\text{AZI}(T) \geq \left(\frac{\lfloor \frac{p}{2} \rfloor + 1}{\lfloor \frac{p}{2} \rfloor^{2}}\right)^{3} + \frac{(\lfloor \frac{p}{2} \rfloor + 1)^{3}}{(\lfloor \frac{p}{2} \rfloor)^{2}} + 8(n-1-p).$$
with equality if and only if $T \cong DS_n([\frac{n-3}{2}], [\frac{n-2}{2}])$. This completes the proof. \hfill $\Box$

**Corollary 3.3** Let $T \in \cup_{2 \leq p \leq n-3} \mathbb{T}_{n,p}$. Then
\[
\text{AZI}(T) \geq \frac{\left( \left\lfloor \frac{n-3}{2} \right\rfloor + 1 \right)^3}{\left( \left\lfloor \frac{n-3}{2} \right\rfloor \right)^2} + \frac{\left( \left\lfloor \frac{n-2}{2} \right\rfloor + 1 \right)^3}{\left( \left\lfloor \frac{n-2}{2} \right\rfloor \right)^2} + 16
\]
with equality if and only if $T \cong DS_n([\frac{n-3}{2}], [\frac{n-2}{2}])$.

**Proof** By Theorem 3.2, it will suffice to show that $\text{AZI}(DS_n([\frac{n-1}{2}], [\frac{n-1}{2}])) > \text{AZI}(DS_n([\frac{n}{2}], [\frac{n}{2}]))$, where $3 \leq p \leq n-3$. By Lemma 3.1, we have
\[
\text{AZI}(DS_n([\frac{p}{2}], [\frac{p}{2}])) = \left( \frac{p}{2} \right) A_{1,\lceil \frac{p}{2} \rceil} + \left( \frac{p}{2} \right) A_{1,\lceil \frac{p}{2} \rceil} + 8(n-1-p)
\]
\[
= \left( \frac{p-1}{2} \right) A_{1,\lceil \frac{p-1}{2} \rceil} + \left( \frac{p-1}{2} \right) A_{1,\lceil \frac{p-1}{2} \rceil} + 8(n-1-p)
\]
\[
< \left( \frac{p-1}{2} \right) A_{1,\lceil \frac{p-1}{2} \rceil} + \left( \frac{p-1}{2} \right) A_{1,\lceil \frac{p-1}{2} \rceil} + 8(n-1-p)
\]
\[
= \text{AZI}(DS_n([\frac{p-1}{2}], [\frac{p-1}{2}])). \hfill \Box
\]

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
\[
\text{AZI}(DS_n([\frac{n-2}{2}], [\frac{n-2}{2}])) < \cdots < \text{AZI}(DS_n(2, n-4)) < \text{AZI}(DS_n(1, n-3)).
\]

**Proof** For $1 \leq p_1 \leq \lfloor \frac{n-2}{2} \rfloor$, note that
\[
\text{AZI}(DS_n(p_1, n-2 - p_1)) = \left( \frac{p_1 + 1}{p_1} \right)^3 + \left( \frac{n-1-p_1}{n-2-p_1} \right)^3 + \left( \frac{p_1 + 1}{n-2-p_1} \right)^3 + \left( \frac{n-1}{n-2-p_1} \right)^3 = f(p_1).
\]
The result follows since the function $f(p_1)$ is increasing for $1 \leq p_1 \leq \lfloor \frac{n-2}{2} \rfloor$. \hfill $\Box$

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

\[\text{Figure 1} \quad T_6^*, T_7^*, T_7^{**}, T_7^{***}\]

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 $\mathbb{T}_6 = \{P_6, T_6^*, DS_6(1,2), DS_6(2,2), DS_6(1,3), S_6\}$,
\[
\text{AZI}(P_6) > \text{AZI}(T_6^*) > \text{AZI}(DS_6(1,2)) > \text{AZI}(DS_6(2,2)) > \text{AZI}(DS_6(1,3)) > \text{AZI}(S_6),
\]
and $\mathbb{T}_7 = \{P_7, T_7^*, DS_7(1,2), T_7^{**}, T_7^{***}, DS_7(1,3), DS_7(2,2), DS_7(2,3), DS_7(1,4), S_7\}$,
\[
\text{AZI}(P_7) > \text{AZI}(T_7^*) > \text{AZI}(DS_7(1,2)) > \text{AZI}(T_7^{**})
\]

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Case 2

From inequalities (3.2)–(3.4) and Theorem 3.5, the inequality 
\[ \text{AZI}(T) < \text{AZI}(DS_n(1, n - 3)), \]
where \( n \geq 8 \).

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

**Theorem 3.5** Let \( T \in T_n \) and \( T \not\cong S_n, DS_n(1, n - 3), DS_n([\frac{n - 3}{2}], [\frac{n - 3}{2}]) \), where \( n \geq 8 \). Then 
\[ \text{AZI}(S_n) < \text{AZI}(DS_n(1, n - 3)) < \text{AZI}(DS_n([\frac{n - 3}{2}], [\frac{n - 3}{2}])) < \text{AZI}(T). \]

**Proof** It is obvious that 
\[ \text{AZI}(S_n) = (n - 3)A_{1, n - 1} + 2A_{1, n - 1} < (n - 3)A_{1, n - 2} + 16 = \text{AZI}(DS_n(1, n - 3)) \]
\[ < [\frac{n - 3}{2}]A_{1, [\frac{n - 3}{2}]+1} + [\frac{n - 3}{2}]A_{1, [\frac{n - 3}{2}]+1} + 16 \]
\[ = \text{AZI}(DS_n([\frac{n - 3}{2}], [\frac{n - 3}{2}])). \]

Since \( T \in T_n \) \( (n \geq 8) \) and \( T \not\cong S_n, DS_n(1, n - 3), DS_n([\frac{n - 3}{2}], [\frac{n - 3}{2}]) \), we consider the following two cases.

**Case 1** \( T \in T_{n-2} \). By Lemma 3.4, we need to prove that 
\[ \text{AZI}(DS_n(2, n - 4)) > \text{AZI}(DS_n([\frac{n - 3}{2}], [\frac{n - 3}{2}])) \]
for \( n \geq 8 \). By Theorem 3.2,
\[ \text{AZI}(DS_n([\frac{n - 3}{2}], [\frac{n - 3}{2}])) < \text{AZI}(DS_n(2, n - 5)) \]
\[ = 2A_{1, 3} + 16 + (n - 5)A_{1, n - 4} \]
\[ < 2A_{1, 3} + A_{3, n - 3} + (n - 4)A_{1, n - 3} \]
\[ = \text{AZI}(DS_n(2, n - 4)). \]

**Case 2** \( T \in \bigcup_{2 \leq p \leq n - 3} T_{n, p} \). By Corollary 3.3, we immediately get
\[ \text{AZI}(DS_n([\frac{n - 3}{2}], [\frac{n - 3}{2}])) < \text{AZI}(T). \]

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 \( G \in G_n \) 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 \( G \in \bigcup_{n - 1 \leq m \leq n} G_{n, m} \). We have the following two cases.

**Case 1** \( G \in G_{n, n - 1} = T_n \) \( (n \geq 5) \). By inequalities (3.2)–(3.4) and Theorem 3.5,
\[ \text{AZI}(DS_n(1, n - 3)) < \text{AZI}(G). \]

**Case 2** \( G \in \bigcup_{n \leq m \leq (\frac{n}{2})} G_{n, m} \). By Corollary 2.2, there exists a graph \( G^* \in G_{n, n - 1} \) 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
\[
AZI(G) \geq AZI(S_n^+) = 24 + (n - 3)A_{1,n-1} \\
> 16 + (n - 3)A_{1,n-2} = AZI(DS_n(1, n - 3)). \quad \Box
\]

4. Unicyclic graphs with the first two smallest AZI indices

Denote by \( C_{n,p} \) the unicyclic graph of order \( n \) formed by attaching \( p \) pendant vertices to a vertex of the cycle \( C_{n-p} \), where \( 0 \leq p \leq n - 3 \). Let \( C_{n,p}^{p_1,p_2, \ldots, p_{n-p}} \) denote the unicyclic graph of order \( n \) obtained from the cycle \( C_{n-p} = v_1v_2 \cdots v_{n-p}v_1 \) by attaching \( p_i \) pendant vertices to vertex \( v_i \), where \( p_i \geq 0 \), \( i = 1, 2, \ldots, n - p \) and \( \sum_{i=1}^{n-p} p_i = p \). Clearly, \( C_{n,0} \cong C_n \), \( C_{n,n-3} \cong S_n^+ \) and \( C_{n,0}^{0,0,\ldots,0} \cong C_{n,p} \).

Let \( U_3^p \) be the unicyclic graph obtained by identifying one vertex of \( C_3 \) and one end vertex of \( P_3 \). Let \( U_n \) be the set of unicyclic graphs of order \( n \geq 3 \). Obviously, \( U_3 = \{K_3\} \), \( U_4 = \{C_4, S_4^+\} \) and \( U_5 = \{C_5, S_5^+, C_5;1, C_5;0,0,0, U_5^0\} \). By simply calculating, we get that \( AZI(S_4^+) < AZI(C_4) \) and \( AZI(S_5^+) < AZI(C_5;1,0) < AZI(C_5) = AZI(U_5^0) \).

Let \( U_{n,p} \) be the set of unicyclic graphs with \( n \) vertices and \( p \) pendant vertices, where \( 0 \leq p \leq n - 3 \). Then \( U_n = \cup_{0 \leq p \leq n-3} U_{n,p} \).

**Lemma 4.1 ([5])** Let \( U \in U_{n,p} \), where \( 0 \leq p \leq n - 3 \). Then
\[
AZI(U) \geq \frac{(p+2)^3}{(p+1)^3} + 8(n-p)
\]
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 \( AZI(C_{n,0}) > AZI(C_{n,1}) > \cdots > AZI(C_{n,n-4}) > AZI(C_{n,n-3}) \).

**Proof** Note that \( AZI(C_{n,p}) = \frac{p(p+2)^3}{(p+3)^3} + 8(n-p) \). 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. \( \Box \)

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

**Corollary 4.3** Let \( U \in \cup_{0 \leq p \leq n-4} U_{n,p} \). Then
\[
AZI(U) \geq \frac{(n-4)(n-2)^3}{(n-3)^3} + 32
\]
with equality if and only if \( U \cong C_{n,n-4} \).

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

**Proof** Since \( U \in U_{n,n-3} \), 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 \( r = (p_1-1)(A_{1,p_1+2}-A_{1,n-2}) + \).
Lemma 5.1
Proof
Observe that

\[ \text{AZI}(U) = \text{AZI}(C_{n,n-4}) = r + A_{1,p_1+2} + A_{p_1+2,p_2+2} - 16. \]  

(4.1)

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

\[ \text{AZI}(U) - \text{AZI}(C_{n,n-4}) = r + A_{1,p_1+2} + A_{p_1+2,p_2+2} - 16. \]  

(4.1)

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

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

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

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

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

\[ \text{AZI}(U) - \text{AZI}(C_{n,n-4}) = r + A_{1,p_1+2} + A_{p_1+2,p_2+2} + A_{p_1+2,p_3+2} + A_{p_2+2,p_3+2} - 32 \]

\[ > 0 + 1 + 3A_{3,3} - 32 = 1 + 3 \cdot \frac{9^3}{4^3} - 32 > 0. \]

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

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 \( U \in U_n \) and \( G \not\cong S_n^+, C_{n,n-4} \), where \( n \geq 6 \). Then

\[ \text{AZI}(S_n^+) < \text{AZI}(C_{n,n-4}) < \text{AZI}(U). \]

5. Bicyclic graphs with the minimum AZI index

Let \( B_n \) be the set of bicyclic graphs of order \( n \geq 4 \). Clearly, \( B_4 = \{K_4 - e\} \). Let \( B_{n,p} \) be the set of bicyclic graphs with \( n \) vertices and \( p \) pendant vertices, where \( 0 \leq p \leq n-4 \). Then \( B_n = \bigcup_{0 \leq p \leq n-4} B_{n,p} \).

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 \( p \) pendant 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 \( B \in B_{n,p} \), where \( 0 \leq p \leq n - 5 \). Then

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

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 \( \text{AZI}(D_{n,r,s,0}) > \text{AZI}(D_{n,r,s,1}) > \cdots > \text{AZI}(D_{n,r,s,n-5}) \).

Proof Observe that

\[ \text{AZI}(D_{n,r,s,p}) = \frac{p(p+4)^3}{(p+3)^3} + 8(n+1-p) := g(p). \]
Then
\[
g'(p) = -7p^4 + 84p^3 + 372p^2 + 704p + 456 \quad (p+3)^4 < 0.
\]
Hence \(g(p)\) is decreasing for \(p \geq 0\). The proof is completed. \(\Box\)

It can be seen from Lemmas 5.1 and 5.2 that

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

Now we consider the set \(B_{n,n-4}\), 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 \(p_1\) pendant 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 \(B_{n,n-4} = \{E_{n}^{p_1,p_2,p_3,p_4}| p_1 \geq p_2 \geq 0, p_3 \geq p_4 \geq 0\ and \ \sum_{i=1}^{4} p_i = n - 4\}\).

**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 \(B \cong E_{n}^{n}^{p_1,p_2,p_3,p_4}\), 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
\[
\text{AZI}(E_{n}^{p_1,p_2,p_3,p_4}) = p_1 A_{1,p_1+3} + p_2 A_{1,p_2+3} + p_3 A_{1,p_3+2} + p_4 A_{1,p_4+2} + A_{p_1+3,p_2+3} + A_{p_1+3,p_3+2} + A_{p_1+3,p_4+2} + A_{p_2+3,p_3+2} + A_{p_2+3,p_4+2}.
\]
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
\[
\text{AZI}(B) - \text{AZI}(E_{n}^{n-4,0,0,0}) = r + A_{p_1+3,p_2+3} + A_{p_1+3,p_3+2} + A_{p_1+3,p_4+2} + A_{p_2+3,p_3+2} + A_{p_2+3,p_4+2} - A_{3,n-1} - 32
\]
\[
> 0 + 16^3 + 12^3 \geq 16 - 27\geq 32 > 0.
\]

**Subcase 1.2** \(p_3 = 0\). Then \(p_4 = 0\). Hence by Lemma 3.1, we have
\[
\text{AZI}(B) - \text{AZI}(E_{n}^{n-4,0,0,0}) = r + A_{p_1+3,p_2+3} - A_{3,n-1}
\]
\[
> 0 + \frac{[p_1 p_2 + 3(n-1)]^3 - [3(n-1)]^3}{n^3} > 0.
\]

**Case 2** \(p_2 = 0\). Let \(q(x) = A_{3,x}\). Then \(q(x)\) is concave increasing for \(x \geq 2\) since
\[
q'(x) = \frac{81 x^2}{(x+1)^4} > 0 \quad \text{and} \quad q''(x) = -\frac{162 x(x-1)}{(x+1)^5} < 0.
\]
It follows that
\[ A_4(\frac{n}{2}) + A_3(\frac{n}{2}) > \cdots > A_3,n-2 + A_3,2, \quad (5.1) \]
\[ A_3(\frac{n+1}{2}) + A_3(\frac{n+1}{2}) > \cdots > A_3,n-1 + A_3,2. \quad (5.2) \]

**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,
\[ AZI(B) = AZI(E_n^{n-4,0,0,0}) \geq r + 3A_{4,3} + 2A_{3,3} - A_{3,n-1} - 32 > 0 + 3 \cdot \frac{123}{5^7} + 2 \cdot \frac{93}{4^3} - 27 - 32 > 0. \]
If $p_1 = 0$, then by Lemma 3.1 and the inequality (5.1), for $n \geq 5$ we have
\[ AZI(B) = AZI(E_n^{n-4,0,0,0}) \]
\[ = r + A_{3,3} + 2(A_{3,p_3+2} + A_{3,p_4+2}) - A_{3,n-1} - 32 \]
\[ > 0 + A_{3,3} + 2(A_{3,n-2} + A_{3,2}) - A_{3,n-1} - 32 \]
\[ = \frac{(n-4)(143n^5 - 3751n^4 - 337n^3 + 5859n^2 - 2484n + 432)}{64n^3(n-1)^3} > 0. \]

**Subcase 2.2** $p_4 = 0$. It follows from Lemma 3.1 and the inequality (5.2) that
\[ AZI(B) = AZI(E_n^{n-4,0,0,0}) \]
\[ = r + (A_{3,p_1+3} + A_{3,p_3+2}) + A_{p_1+3,3} - A_{3,n-1} = 16 \]
\[ \geq 0 + (A_{3,n-1} + A_{3,2}) + A_{p_1+3,3} - A_{3,n-1} = 16 \]
\[ = A_{p_1+3,3} + 2 = 8 \geq 0 \]
with equality if and only if $p_1 = n - 4$ and $p_2 = p_3 = p_4 = 0$, that is, $B = E_n^{n-4,0,0,0}$. \qed

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 $AZI(D_{n,3,3,n-5}) < AZI(B)$.

**Proof** Note that $\mathbb{B}_n = \bigcup_{0 \leq p \leq n-4} \mathbb{B}_{n,p}$. Then by Corollary 5.3 and Lemma 5.4, it will suffice to prove that for $n \geq 5$, $AZI(D_{n,3,3,n-5}) < AZI(E_n^{n-4,0,0,0})$. It is obvious that
\[ AZI(E_n^{n-4,0,0,0}) - AZI(D_{n,3,3,n-5}) = \frac{27(n-1)^3}{n^3} + \frac{(n-1)^3}{(n-2)^3} - 16 > 0. \]
This completes the proof of Theorem 5.5. \qed

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**References**