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Unicyclic and bicyclic graphs with minimal augmented Zagreb index

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Abstract

The augmented Zagreb index of a graph G is defined as

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

where $E(G)$ is the edge set, and d_u, d_v are the degrees of vertices u and v in G, respectively. This new molecular structure descriptor, introduced by Furtula *et al.* (J. Math. Chem. 48:370-380, 2010), has proven to be a valuable predictive index in the study of the heat of formation in heptanes and octanes. In this paper, the n-vertex unicyclic graphs with the minimal and the second minimal *AZI* indices and the n-vertex bicyclic graphs with the minimal *AZI* index are determined.

MSC: 05C35; 05C75; 92E10

Keywords: augmented Zagreb index; extremal graphs; unicyclic graphs; bicyclic graphs

1 Introduction

Let $G = (V, E)$ be a simple, finite and undirected graph of order $n = |V|$ and size $m = |E|$. For $v \in V(G)$, the degree of v, denoted by d_v, is the number of edges incident to v. A vertex of degree one is said to be a pendent vertex. The maximum vertex degree is denoted by Δ, the minimum vertex degree is denoted by δ, and the minimum non-pendent vertex degree is denoted by δ_1. If u and v are two adjacent vertices of G, then the edge connecting them will be denoted by uv [1]. Other notations used in this work are standard and mainly taken from [1–3].

A description of the structure or shape of molecules is very helpful in predicting the activity and properties of molecules in complex experiments. Molecular descriptors play a significant role in mathematical chemistry, especially in QSPR/QSAR investigations. Among them, topological indices [4] play an important role. Today, many topological indices exist that have various applications in chemistry [2, 5, 6]. Here, a relatively new topological index is considered. In 2010, Furtula *et al.* [7] proposed a new, vertex-degree-based graph topological index called the augmented Zagreb index (AZI), defined as

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

and showed that it is a valuable predictive index in the study of the heat of formation in heptanes and octanes. Moreover, Gutman and Tošovič [8] recently tested the correlation abilities of 20 vertex-degree-based topological indices for the case of standard heats of formation and normal boiling points of octane isomers. They found that the AZI index yields the best results. Consequently, the AZI index should be preferred in designing quantitative, structure-property relations.

Furtula *et al.* [7] obtained several tight upper and lower bounds of the AZI index of a chemical tree and showed that among all trees, the star graph has the minimal AZI value. Huang *et al.* [9] and Wang *et al.* [10] provided particular bounds on the AZI indices of connected graphs and characterized the corresponding extremal graphs. Ali *et al.* [11] established inequalities between AZI and several other vertex-degree-based topological indices. Ali *et al.* [12] proposed tight upper bounds for the AZI of chemical bicyclic and unicyclic graphs and provided a Nordhaus-Gaddum-type result for the AZI index.

In this paper, the n-vertex unicyclic graphs are determined with the minimal and the second minimal AZI indices. Additionally, the n-vertex bicyclic graphs in which the AZI index attains its minimal value are obtained.

2 Preliminaries

Some of the auxiliary results provided below will be used in the main theorem proofs. For convenience, let $A(x,y) = (\frac{xy}{x+y-2})^3$ for $x, y \geq 1$ with $x + y > 2$. Obviously, $A(x,y) = A(y,x)$.

Lemma 2.1 ([9])

(i) *$A(1,y)$ is decreasing for $y \geq 2$.*

(ii) *$A(2,y) = 8$.*

(iii) *If $y \geq 3$ is fixed, then $A(x,y)$ is increasing for $x \geq 3$.*

Lemma 2.2 ([9]) *$A(1,\Delta) \leq A(1,i) \leq A(1,2) = A(2,j) < A(3,3) \leq A(k,l) \leq A(\Delta,\Delta)$, where $2 \leq i,j \leq \Delta$ and $3 \leq k \leq l \leq \Delta$.*

Lemma 2.3 *Let $f(x) = xA(1,x+2) - (x+1)A(1,x+3)$ with $x > 0$. Then $f(x)$ increases in x.*

Proof Let $h(x) = xA(1,x+2) = \frac{x(x+2)^3}{(x+1)^3}$. Therefore, $f(x) = h(x) - h(x+1)$.

Then

$$h'(x) = \frac{(x+2)^2(x^2+2)}{(x+1)^4}$$

and

$$h''(x) = -\frac{12(x+2)}{(x+1)^5} < 0.$$

Applying Lagrange's mean value theorem, $f'(x) = h'(x) - h'(x+1) = -h''(\xi) > 0$ with $x \leq \xi \leq x+1$. Therefore, $f(x)$ increases in x, which completes the proof. □

Lemma 2.4 *Let $g(x,y) = A(x,y) - A(x-1,y)$, with x and y as positive integers, and $y < x+2$. Then $g(x,y)$ strictly decreases in x for fixed $y \geq 2$.*

Proof First, the partial derivative $g(x,y)$ is considered with respect to x,

$$\frac{\partial g(x,y)}{\partial x} = 3y^3(y-2)\left(\frac{x}{(x+y-2)^2}+\frac{x-1}{(x+y-3)^2}\right)\left(\frac{x}{(x+y-2)^2}-\frac{x-1}{(x+y-3)^2}\right).$$

Now, we will show that

$$\frac{x}{(x+y-2)^2}-\frac{x-1}{(x+y-3)^2} < 0.$$

Let $m_1(t) = \frac{t}{(t+y-2)^2}$ for $y-t<2$. Then the function $m_1(t)$ decreases in t because

$$m_1'(t) = \frac{y-2-t}{(t+y-2)^3} < 0.$$

Therefore, $\frac{\partial g(x,y)}{\partial x} < 0$, from which it follows that $g(x,y)$ strictly decreases in x. □

Lemma 2.5 *Let $l_1(x) = 2A(x-2,3) - A(x-1,3)$ for $x \geq 5$. Then $l_1(x) > 8$.*

Proof From the definition of $A(x,y)$, the following is obtained:

$$l_1(x) = 27 \times \left(\frac{2(x-2)^3}{(x-1)^3}-\frac{(x-1)^3}{x^3}\right).$$

Therefore,

$$l_1'(x) = 81 \times \frac{(\sqrt{2}-1)x^3+(3-2\sqrt{2})x^2-3x+1}{(x-1)^2x^2} \times \left(\frac{\sqrt{2}(x-2)}{(x-1)^2}+\frac{x-1}{x^2}\right).$$

$l_1'(x) > 0$ must be demonstrated. Let $m_2(t) = (\sqrt{2}-1)t^3 + (3-2\sqrt{2})t^2 - 3t + 1$, so $m_2'(t) = 3(\sqrt{2}-1)t^2 + 2(3-2\sqrt{2})t - 3$, which is positive for $t \geq 5$, implying that $m_2(t)$ is an increasing function for t. Thus, $m_2(t) \geq m_2(5) > 0$. Therefore, $l'(x) > 0$ and $l_1(x) \geq l_1(5) = 8.95725 > 8$. □

Lemma 2.6 *Let $l_2(x) = (\frac{3(x+2)}{x+3})^3 + (\frac{3(n-x-2)}{n-x-1})^3$, where $n \geq 6$ and $0 \leq x \leq n-4$. Then $l_2(x) \geq (\frac{3(n+1)}{n+4})^3 + (\frac{3(2n-1)}{2n+2})^3$.*

Proof Consider the derivative $l_2(x)$ with respect to x,

$$l_2'(x) = 3^4 \times \left(\frac{(x+2)(n-x-1)^2+(x+3)^2(n-x-2)}{(x+3)^2(n-x-1)^2}\right) \times \left(\frac{(x+2)(n-x-1)^2-(x+3)(n-x-2)^2}{(x+3)^2(n-x-1)^2}\right).$$

Now, the expression $(x+2)(n-x-1)^2-(x+3)(n-x-2)^2$ must be discussed. Let $m_3(t) = (t+2)(n-t-1)^2$ with $0 \leq t \leq n-4$. Then $m_3(t) - m_3(t+1) = (t+2)(n-t-1)^2 - (t+3)(n-t-2)^2$ and $m_3'(t) = (n-t-1)(n-3t-5)$. Obviously, $n-t-1 > 0$.

If $t > \frac{n-5}{3}$, then $m_3'(t) < 0$, implying that $m_3(t)$ is decreasing for t. Therefore, $l_2'(x) > 0$ and $l_2(x) \geq l_2(\frac{n-5}{3})$.

If $t < \frac{n-5}{3}$, then $m_3'(t) > 0$, implying $m_3(t) < m_3(t+1)$. Therefore, $l_2'(x) < 0$ and $l_2(x) \geq l_2(\frac{n-5}{3})$.

Therefore, $l_2(x) \geq (\frac{3(n+1)}{n+4})^3 + (\frac{3(2n-1)}{2n+2})^3$ for $0 \leq x \leq n-4$. □

Lemma 2.7 *Let* $l_3(x) = 2(\frac{3(x+1)}{x+4})^3 - (\frac{3(x-1)}{x})^3$, *where* $x \geq 6$. *Then* $l_3(x) \geq l_3(6)$.

Proof We have

$$l_3'(x) = 3^4 \times \left(\frac{\sqrt{6}(x+1)}{(x+4)^2} + \frac{x-1}{x^2}\right)\left(\frac{\sqrt{6}(x+1)x^2 - (x-1)(x+4)^2}{(x+4)^2 x^2}\right).$$

Let $m_4(t) = \sqrt{6}(t+1)t^2 - (t-1)(t+4)^2$ for $t \geq 6$. It is easily seen that $m_4'(t) = 3(\sqrt{6}-1)t^2 + 2(\sqrt{6}-7)t - 8$. By simple calculation, $m_4'(t) > 0$ for $t \geq 6$. Then $m_4(t) \geq m_4(6) > 0$ and $l_3'(x) > 0$, implying that $l_3(x)$ is increasing in x. Therefore, $l_3(x) \geq l_3(6)$ for $x \geq 6$. □

3 On the *AZI* indices of unicyclic graphs

In this section, the n-vertex unicyclic graphs are determined with the minimal and the second minimal *AZI* indices. The technique from [13] is used for these determinations.

For $r \neq s$, a graph G is said to be (r,s)-biregular if each vertex has degree r or s, and each vertex of degree r is adjacent to some vertices of degree s and vice versa. Let ϕ_1 be the class of connected graphs whose pendent vertices are adjacent to the vertices of maximum degree and all other edges have at least one end-vertex of degree two. Let ϕ_2 be the class of connected graphs with vertices that are of degree at least two. Additionally, all of the edges have at least one end-vertex of degree two.

Lemma 3.1 ([10]) *Let* G *be a connected graph of order* $n \geq 3$ *with* m *edges,* p *pendent vertices, maximum degree* Δ *and minimum non-pendent vertex degree* δ_1. *Then*

$$\mathrm{AZI}(G) \geq p\left(\frac{\Delta}{\Delta-1}\right)^3 + (m-p)\left(\frac{\delta_1^2}{2\delta_1-2}\right)^3$$

with equality if and only if G *is isomorphic to a* $(1,\Delta)$*-biregular graph or* G *is isomorphic to a regular graph or* $G \in \phi_1$ *or* $G \in \phi_2$.

Let $\mathscr{U}_n$ be the set of n-vertex unicyclic graphs. Let $\mathscr{U}_{n,p}$ be the set of unicyclic graphs with n vertices and p pendent vertices, and let $C_{n,p}$ be the unicyclic graph formed from C_{n-p} by attaching p pendent vertices to a vertex of the cycle C_{n-p}, where $0 \leq p \leq n-3$. Clearly $C_{n-p,0} = C_n$.

Lemma 3.2 ([9]) *Let* $G \in \mathscr{U}_{n,p}$, *where* $0 \leq p \leq n-3$. *Then*

$$\mathrm{AZI}(G) \geq p\left(\frac{p+2}{p+1}\right)^3 + 8(n-p)$$

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

Lemma 3.3 *For every positive integer n, graphs $C_{n,p}$ with $0 \leq p \leq n-3$, it holds that*

$$\mathrm{AZI}(C_{n,n-3}) < \mathrm{AZI}(C_{n,n-4}) < \cdots < \mathrm{AZI}(C_{n,1}) < \mathrm{AZI}(C_{n,0}).$$

Proof Consider the function

$$f_1(x) = x\left(\frac{x+2}{x+1}\right)^3 + 8(n-x) \quad \text{for } 0 \leq x \leq n-3.$$

Then

$$f_1'(x) = -\frac{x(7x^3+28x^2+42x+24)}{(x+4)^4} < 0 \quad \text{as } x \geq 1.$$

Thus, $f(x)$ is a decreasing function for $1 \leq x \leq n-3$. Because $f_1(1) = 8n - \frac{37}{8}$ and $f_1(0) = 8n$, then

$$\mathrm{AZI}(C_{n,n-3}) < \mathrm{AZI}(C_{n,n-4}) < \cdots < \mathrm{AZI}(C_{n,1}) < \mathrm{AZI}(C_{n,0}). \qquad \square$$

Theorem 3.4 *Among all graphs in $\mathscr{U}_n$ with $n \geq 3$, $C_{n,n-3}$ is the unique graph with the minimal AZI index, which is equal to* $\frac{(n-3)(n-1)^3}{(n-2)^3} + 24$.

Proof By Lemma 3.1 and Lemma 3.2, $C_{n,p}$ is attained and is the unique graph with the minimal *AZI* index among all graphs in $\mathscr{U}_{n,p}$ with $0 \leq p \leq n-3$. Applying Lemma 3.3, $C_{n,n-3}$ is the unique graph with the minimal *AZI* index in $\mathscr{U}_n$. It is clear that $\mathrm{AZI}(C_{n,n-3}) = \frac{(n-3)(n-1)^3}{(n-2)^3} + 24$. $\square$

The vertices of C_3 are consecutively labeled by v_1, v_2, v_3. Let $Q_n(n_1, n_2, n_3)$ be the unicyclic graph formed by attaching n_i pendent vertices to v_i, where $n_i \geq 0$ for $i = 1, 2, 3$, $n_1 \geq n_2 \geq n_3$, and $\sum_{i=1}^{3} n_i = n-3$.

Lemma 3.5 *Let $G \cong Q_n(n_1, n_2, n_3)$ with $n_1 \geq n_2 \geq 1$ and $G' \cong Q_n(n_1+1, n_2-1, n_3)$ (see Figure* 1*). Then* $\mathrm{AZI}(G') < \mathrm{AZI}(G)$.

Proof Consider the transformation σ depicted in Figure 1. By applying the transformation σ to G, a pendent edge is cut from v_2 and attached to v_1. By Lemma 2.3 and Lemma 2.4,

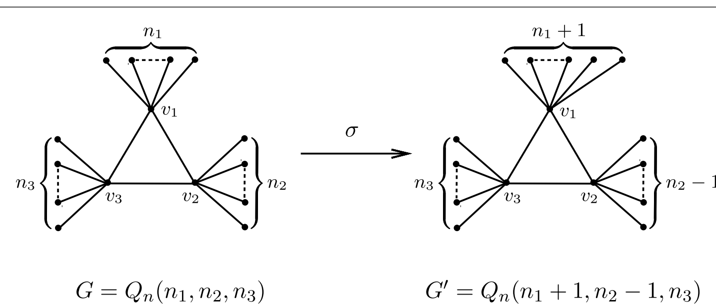


Figure 1 Transformation σ from Lemma 3.5.

the change of the *AZI* index after applying this transformation is

$$\begin{aligned}
&\mathrm{AZI}(G) - \mathrm{AZI}(G') \\
&\quad = n_1 A(1, n_1 + 2) + n_2 A(1, n_2 + 2) + A(n_1 + 2, n_2 + 2) + A(n_1 + 2, n_3 + 2) \\
&\qquad + A(n_2 + 2, n_3 + 2) - \bigl[(n_1 + 1)A(1, n_1 + 3) + (n_2 - 1)A(1, n_2 + 1) \\
&\qquad + A(n_1 + 3, n_2 + 1) + A(n_1 + 3, n_3 + 2) + A(n_2 + 1, n_3 + 2)\bigr] \\
&\quad = \bigl[n_1 A(1, n_1 + 2) - (n_1 + 1)A(1, n_1 + 3)\bigr] - \bigl[(n_2 - 1)A(1, n_2 + 1) \\
&\qquad - n_2 A(1, n_2 + 2)\bigr] + \bigl[A(n_1 + 2, n_2 + 2) - A(n_1 + 3, n_2 + 1)\bigr] \\
&\qquad + \bigl[A(n_2 + 2, n_3 + 2) - A(n_2 + 1, n_3 + 2)\bigr] \\
&\qquad - \bigl[A(n_1 + 3, n_3 + 2) - A(n_1 + 2, n_3 + 2)\bigr] \\
&\quad = f(n_1) - f(n_2 - 1) + A(n_1 + 2, n_2 + 2) - A(n_1 + 3, n_2 + 1) \\
&\qquad + g(n_2 + 2, n_3 + 2) - g(n_1 + 3, n_3 + 2).
\end{aligned}$$

By Lemma 2.3, the expression $f(n_1) - f(n_2 - 1)$ is positive for $n_1 > n_2 - 1$. By Lemma 2.4, $g(n_2 + 2, n_3 + 2) > g(n_1 + 3, n_3 + 2)$ for $n_1 \geq n_2 \geq n_3$. Note that $(n_1 + 2)(n_2 + 2) > (n_1 + 3)(n_2 + 1)$, so

$$\frac{(n_1 + 2)^3 (n_2 + 2)^3}{(n_1 + n_2 + 2)^3} > \frac{(n_1 + 3)^3 (n_2 + 1)^3}{(n_1 + n_2 + 2)^3},$$

that is, $A(n_1 + 2, n_2 + 2) > A(n_1 + 3, n_2 + 1)$. Thus, it has been shown that after the transformation σ, the *AZI* index of G decreases. □

Theorem 3.6 *Among all graphs in $\mathscr{U}_n$ with $n \geq 4$.*

(i) *For $n = 4$ or $n \geq 6$, $C_{n,n-4}$ is the unique graph with the second minimal AZI index, which is equal to $(n - 4)(\frac{n-2}{n+1})^3 + 32$.*
(ii) *For $n = 5$, $Q_5(1,1,0)$ is the unique graph with the second minimal AZI index, which is equal to $\frac{2{,}185}{64}$.*

Proof By Lemma 3.2 and Lemma 3.3, the second minimal *AZI* index of graphs in $\mathscr{U}_n$ with $n \geq 4$ is achieved by the graphs in $\mathscr{U}_{n,n-3} \setminus \{C_{n,n-3}\}$ and $C_{n,n-4}$. Now, two cases are considered.

Case 1. $n = 4$.

Obviously, C_4 is the unique graph with the second minimal *AZI* index, which is equal to 32.

Case 2. $n \geq 5$.

Note that $n_3 \geq 1$, so $n_2 \geq n_3 \geq 1$. By Lemma 3.5, it is determined that $Q_n(n - 4, 1, 0)$ is the unique graph with the minimal *AZI* index among all of the graphs in $\mathscr{U}_{n,n-3} \setminus \{C_{n,n-3}\}$. Note that

$$\begin{aligned}
\mathrm{AZI}\bigl(Q_n(n - 4, 1, 0)\bigr) &= (n - 4)A(1, n - 2) + A(1, 3) + A(2, n - 2) \\
&\quad + A(2, 3) + A(3, n - 2)
\end{aligned}$$

and

$$\mathrm{AZI}(C_{n,n-4}) = (n-4)A(1,n-2) + 2A(2,n-2) + 2A(2,2).$$

Then

$$\begin{aligned}\mathrm{AZI}\big(Q_n(n-4,1,0)\big) - \mathrm{AZI}(C_{n,n-4}) &= A(3,n-2) + A(1,3) - 16 \\ &= A(3,n-2) - \frac{101}{8}.\end{aligned}$$

By Lemma 2.1(iii), $A(3,n-2)$ is increasing for $n \geq 5$. Using a simple calculation, it can be shown that $\mathrm{AZI}(Q_5(1,1,0)) < \mathrm{AZI}(C_{5,1})$ for $n = 5$ and $\mathrm{AZI}(Q_n(n-4,1,0)) > \mathrm{AZI}(C_{n,n-4})$ for $n \geq 6$.

Thus, it follows that $Q_5(1,1,0)$ for $n = 5$ is the unique graph with the second minimal *AZI* index, which is equal to $\frac{2{,}185}{64}$, and $C_{n,n-4}$ for $n \geq 6$ is the unique graph with the second minimal *AZI* index, which is equal to $(n-4)(\frac{n-2}{n+1})^3 + 32$. □

4 On the *AZI* indices of bicyclic graphs

In this section, the n-vertex bicyclic graphs are determined with the minimal *AZI* index for $n \geq 5$.

Let $\mathscr{B}_{n,p}$ be the set of bicyclic graphs with n vertices and p pendent vertices for $0 \leq p \leq n-4$. Let $D_{n,p}^{r,t}$ be the n-vertex bicyclic graph by identifying one vertex of two cycles C_r and C_t and attaching p pendent vertices to the common vertex, where $r \geq t \geq 3$ and $0 \leq p \leq n-5$.

Lemma 4.1 ([9]) *Let G be a bicyclic graph with $n \geq 5$ vertices and p pendent vertices, where $0 \leq p \leq n-5$. Then*

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

with equality holding if and only if $G \cong D_{n,p}^{r,t}$, where $r \geq t \geq 3$.

Let $\mathscr{D}_{n,p}$ be the set of graphs $D_{n,p}^{r,t}$ with $3 \leq t \leq r \leq n-p-2$ and $r + t = n-p+1$. Let $D_{n,p}$ be any graph in $\mathscr{D}_{n,p}$.

Lemma 4.2 *For the graphs in $\mathscr{D}_{n,p}$ with $0 \leq p \leq n-5$ and $n \geq 5$, it holds that*

$$\mathrm{AZI}(D_{n,n-5}) < \mathrm{AZI}(D_{n,n-6}) < \cdots < \mathrm{AZI}(D_{n,1}) < \mathrm{AZI}(D_{n,0}).$$

Proof Let $H(x) = \frac{x(x+4)^3}{(x+3)^3} + 8(n-x+1)$, where $0 \leq x \leq n-5$.

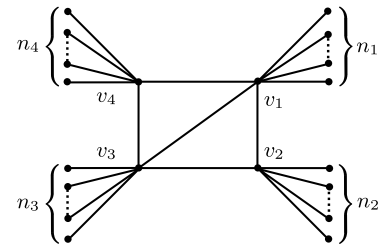
Note that

$$H'(x) = \frac{(x+4)^2(x^2+4x+12) - 8(x+3)^4}{(x+3)^4} < 0.$$

Thus, $H(x)$ is decreasing for x. The result follows. □

Let C_4^* be the bicyclic graph obtained by adding an edge to the cycle C_4. Label the vertices of C_4^* by v_1, v_2, v_3, v_4 with $d_{v_1} = d_{v_3} = 3$, $d_{v_2} = d_{v_4} = 2$, respectively. Let $S_n(n_1, n_2, n_3, n_4)$

Figure 2 Graph $S_n(n_1, n_2, n_3, n_3)$.



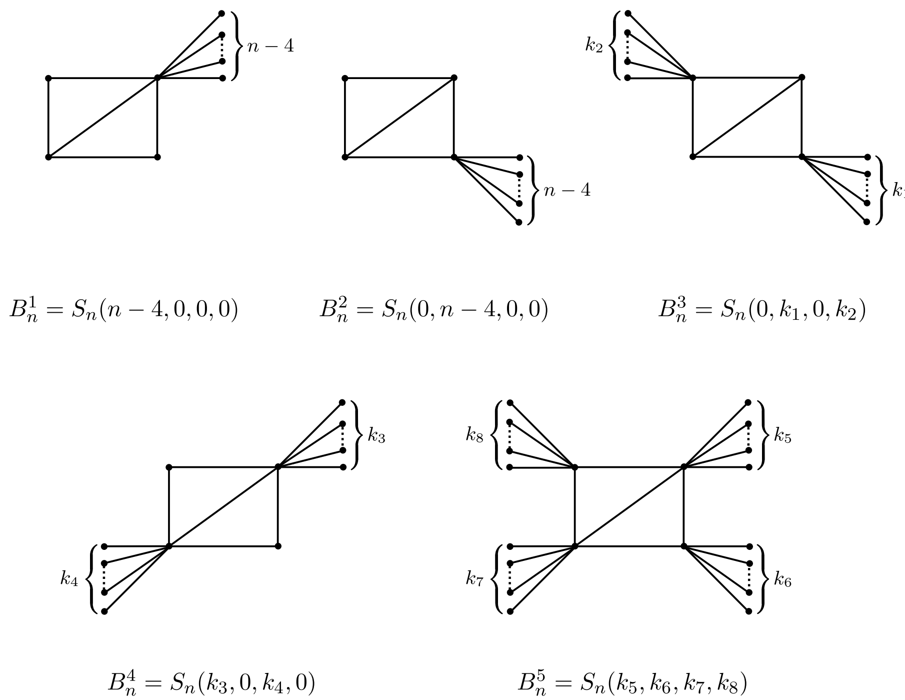


Figure 3 Graphs B_n^1, B_n^2, B_n^3, B_n^4 and B_n^5.

be the graph formed from C_4^* by attaching n_i pendent vertices to v_i, where $n_i \geq 0$ for $i = 1,2,3,4$, $n_1 \geq n_3$, $n_2 \geq n_4$ and $\sum_{i=1}^4 n_i = n-4$ (see Figure 2). For convenience, let $B_n^1 \cong S_n(n-4,0,0,0)$, $B_n^2 \cong S_n(0,n-4,0,0)$, $B_n^3 \cong S_n(0,k_1,0,k_2)$ with $k_1+k_2 = n-4$, $B_n^4 \cong S_n(k_3,0,k_4,0)$ with $k_3+k_4 = n-4$ and $B_n^5 \cong S_n(k_5,k_6,k_7,k_8)$ with $k_5+k_6+k_7+k_8 = n-4$ (see Figure 3).

Lemma 4.3 *Let $G \in \mathscr{B}_{n,n-4}$ with $n \geq 5$. Then*

$$\mathrm{AZI}(G) \geq (n-4)\left(\frac{n-1}{n-2}\right)^3 + \left(\frac{3(n-1)}{n}\right)^3 + 32$$

with equality if and only if $G \cong S_n(n-4,0,0,0)$.

Proof For $n = 5$, $G \cong S_5(1,0,0,0)$ or $G \cong S_5(0,1,0,0)$.

From the definition of the *AZI* index, the following is obtained:

$$\mathrm{AZI}\big(S_5(1,0,0,0)\big) = A(1,4) + 2A(4,2) + A(4,3) + 2A(3,2)$$

and

$$\mathrm{AZI}\big(S_5(0,1,0,0)\big) = A(1,3) + 3A(3,3) + 2A(3,2).$$

By simple calculation, $\mathrm{AZI}(S_5(1,0,0,0)) < \mathrm{AZI}(S_5(0,1,0,0))$. Lemma 4.3 obviously holds.

For $n \geq 6$, G is isomorphic to one of the graphs B_n^1, B_n^2, B_n^3, B_n^4, B_n^5 shown in Figure 3. By the definition of the *AZI* index,

$$\begin{aligned}
\mathrm{AZI}\big(B_n^1\big) &= (n-4)A(1,n-1) + 2A(2,n-1) + A(3,n-1) + 2A(2,3), \\
\mathrm{AZI}\big(B_n^2\big) &= (n-4)A(1,n-2) + 2A(3,n-2) + A(3,3) + 2A(2,3), \\
\mathrm{AZI}\big(B_n^3\big) &= k_1A(1,k_1+2) + k_2A(1,k_2+2) + 2A(3,k_1+2) \\
&\quad + 2A(3,k_2+2) + A(3,3), \\
\mathrm{AZI}\big(B_n^4\big) &= k_3A(1,k_3+3) + k_4A(1,k_4+3) + 2A(2,k_3+3) \\
&\quad + 2A(2,k_4+3) + A(k_3+3,k_4+3)
\end{aligned}$$

and

$$\begin{aligned}
\mathrm{AZI}\big(B_n^5\big) &= k_5A(1,k_5+3) + k_6A(1,k_6+2) + k_7A(1,k_7+3) \\
&\quad + k_8A(1,k_8+2) + A(k_5+3,k_6+2) + A(k_5+3,k_8+2) \\
&\quad + A(k_5+3,k_7+3) + A(k_7+3,k_8+2) + A(k_7+3,k_6+2).
\end{aligned}$$

Claim 1 $\mathrm{AZI}(B_n^1) < \mathrm{AZI}(B_n^2)$.

Using Lemma 2.2 and Lemma 2.5, we get

$$\begin{aligned}
\mathrm{AZI}\big(B_n^2\big) - \mathrm{AZI}\big(B_n^1\big) &= (n-4)\big(A(1,n-2) - A(1,n-1)\big) \\
&\quad + \big(2A(n-2,3) - A(n-1,3) - A(3,2)\big) \\
&\quad + \big(A(3,3) - A(3,2)\big) > 0.
\end{aligned}$$

This proves Claim 1.

Claim 2 $\mathrm{AZI}(B_n^1) < \mathrm{AZI}(B_n^3)$.

Note that $k_1 + k_2 = n - 4$. Using Lemma 2.1, Lemma 2.2, Lemma 2.6 and Lemma 2.7, we have

$$\begin{aligned}
&\mathrm{AZI}\big(B_n^3\big) - \mathrm{AZI}\big(B_n^1\big) \\
&\quad = k_1A(1,k_1+2) + k_2A(1,k_2+2) - (n-4)A(1,n-1) + 2\big(A(k_1+2,3) \\
&\qquad + A(k_2+2,3)\big) - A(n-1,3) + A(3,3) - 4A(3,2) \\
&\quad \geq k_1A(1,n-2) + k_2A(1,n-2) - (n-4)A(1,n-1) + 2\big(A(k_1+2,3) \\
&\qquad + A(k_2+2,3)\big) - A(n-1,3) + A(3,3) - 4A(3,2)
\end{aligned}$$

$$
\begin{aligned}
&= (n-4)\bigl(A(1,n-2)-A(1,n-1)\bigr)+2\bigl(A(k_1+2,3)+A(k_2+2,3)\bigr) \\
&\quad - A(n-1,3)+A(3,3)-4A(3,2) \\
&> 2\bigl(A(k_1+2,3)+A(k_2+2,3)\bigr)-A(n-1,3)+A(3,3)-4A(3,2) \\
&> 2\left(\frac{3(n+1)}{n+4}\right)^3-\left(\frac{3(n-1)}{n}\right)^3 \\
&\quad +2\left(\frac{3(2n-1)}{2n+2}\right)^3+\left(\frac{9}{4}\right)^3-4\times 2^3 \\
&\geq l_3(6)+2\times 3^3\times\left(\frac{2n-1}{2n+2}\right)^3+\left(\frac{9}{4}\right)^3-4\times 2^3.
\end{aligned}
$$

Let $q(x)=(\frac{2x-1}{2x+2})^3$, so $q'(x)=\frac{9(2x-1)^2}{(2x+2)^4}>0$, implying that $q(x)$ is strictly increasing for x. Then

$$
\begin{aligned}
\mathrm{AZI}\bigl(B_n^3\bigr)-\mathrm{AZI}\bigl(B_n^1\bigr) &> 2\left(\frac{3\times 7}{10}\right)^3-\left(\frac{3\times 5}{6}\right)^3+2\times 3^3\times\left(\frac{11}{14}\right)^3 \\
&\quad +\left(\frac{9}{4}\right)^3-4\times 2^3>0.
\end{aligned}
$$

This proves Claim 2.

Claim 3 $\mathrm{AZI}(B_n^1)<\mathrm{AZI}(B_n^4)$.

Because $k_3+k_4=n-4$, using Lemma 2.1 and Lemma 2.2, we have

$$
\begin{aligned}
&\mathrm{AZI}\bigl(B_n^4\bigr)-\mathrm{AZI}\bigl(B_n^1\bigr) \\
&\quad = k_3A(1,k_3+3)+k_4A(1,k_4+3)-(n-4)A(1,n-1) \\
&\qquad + A(k_3+3,k_4+3)-A(n-1,3) \\
&\quad > \left(\frac{(k_3+3)(k_4+3)}{k_3+k_4+4}\right)^3-\left(\frac{3(n-1)}{n}\right)^3 \\
&\quad = \left(\frac{k_3k_4+3(n-4)+9}{n}\right)^3-\left(\frac{3(n-1)}{n}\right)^3 \quad \text{as } k_3+k_4=n-4 \\
&\quad > 0.
\end{aligned}
$$

This proves Claim 3.

Claim 4 $\mathrm{AZI}(B_n^1)<\mathrm{AZI}(B_n^5)$.

The following two cases are presented.

Case 1. $k_5\geq 2$, $k_6\geq 2$.

Using Lemma 2.1 and Lemma 2.2, it follows that

$$
\begin{aligned}
\mathrm{AZI}\bigl(B_n^5\bigr) &> k_5A(1,n-2)+k_6A(1,n-2)+k_7A(1,n-2)+k_8A(1,n-2) \\
&\quad +A(5,4)+A(5,3)+A(5,2)+A(3,2)+A(3,4)
\end{aligned}
$$

$$
\begin{aligned}
&> (n-4)A(1,n-1) + \left(\frac{20}{7}\right)^3 + \left(\frac{5}{2}\right)^3 + \left(\frac{12}{5}\right)^3 + 2\times 2^3 \\
&> (n-4)A(1,n-1) + 2\times 2^3 + 3^3 + 2\times 2^3 \\
&> (n-4)A(1,n-1) + 3^3 \times \left(\frac{n-1}{n}\right)^3 + 4\times 2^3 \\
&= (n-1)A(1,n-1) + A(3,n-1) + 2A(n-1,2) + 2A(3,2) \\
&= \mathrm{AZI}\left(B_n^1\right).
\end{aligned}
$$

Case 2. $k_5 = 2$, $k_6 = 1$ or $k_5 = 1$, $k_6 = 2$ or $k_5 = 1$, $k_6 = 1$.

If $k_5 = 2$ and $k_6 = 1$, then according to the definition of graph $S_n(n_1, n_2, n_3, n_4)$, $B_n^5 \cong S_7(2,1,0,0)$ or $S_8(2,1,1,0)$ or $S_8(2,1,0,1)$ or $S_9(2,1,1,1)$ or $S_9(2,1,2,0)$ or $S_{10}(2,1,2,1)$.

By the definition of the *AZI* index and some calculations, the following are obtained:

$$
\begin{aligned}
&\mathrm{AZI}\left(S_7(2,1,0,0)\right) \doteq 65.922 > \mathrm{AZI}\left(B_7^1\right) \doteq 54.187, \\
&\mathrm{AZI}\left(S_8(2,1,1,0)\right) \doteq 78.424 > \mathrm{AZI}\left(B_8^1\right) \doteq 56.440, \\
&\mathrm{AZI}\left(S_8(2,1,0,1)\right) \doteq 80.313 > \mathrm{AZI}\left(B_8^1\right) \doteq 56.440, \\
&\mathrm{AZI}\left(S_9(2,1,1,1)\right) \doteq 95.248 > \mathrm{AZI}\left(B_9^1\right) \doteq 58.427, \\
&\mathrm{AZI}\left(S_9(2,1,2,0)\right) \doteq 88.955 > \mathrm{AZI}\left(B_9^1\right) \doteq 58.427
\end{aligned}
$$

and

$$
\mathrm{AZI}\left(S_{10}(2,1,2,1)\right) \doteq 107.580 > \mathrm{AZI}\left(B_{10}^1\right) \doteq 60.226.
$$

In a similar way, we can verify the inequality $\mathrm{AZI}(B_n^1) < \mathrm{AZI}(B_n^5)$ for each of the cases for $k_5 = 1$, $k_6 = 2$ or $k_5 = 1$, $k_6 = 1$. The details are omitted. This proves Claim 4.

Thus, the result follows from Claims 1-4. □

Theorem 4.4 *For the graphs in* $\mathscr{B}_n$ *with* $n \geq 5$, *it holds that* $D_{n,n-5}^{3,3}$ *is the unique graph with the minimal AZI index, which is equal to* $(n-5)(\frac{n-1}{n-2})^3 + 48$.

Proof Using Lemma 4.3, among all of the graphs in $\mathscr{B}_{n,n-4}$, $S_n(n-4,0,0,0)$ is the unique graph with the minimal *AZI* index, which is equal to $(n-4)(\frac{n-1}{n-2})^3 + (\frac{3(n-1)}{n})^3 + 32$. Using Lemma 4.1 and Lemma 4.2, among all of the graphs in $\mathscr{B}_{n,p}$ with $0 \leq p \leq n-5$, $D_{n,n-5}^{3,3}$ is the unique graph with the minimal *AZI* index, which is equal to $(n-5)(\frac{n-1}{n-2})^3 + 48$.

Note that

$$
\begin{aligned}
&\mathrm{AZI}\left(S_n(n-4,0,0,0)\right) - \mathrm{AZI}\left(D_{n,n-5}^{3,3}\right) \\
&\quad = (n-4)\left(\frac{n-1}{n-2}\right)^3 + \left(\frac{3(n-1)}{n}\right)^3 \\
&\qquad + 32 - (n-5)\left(\frac{n-1}{n-2}\right)^3 - 48 \\
&\quad = \left(\frac{n-1}{n-2}\right)^3 + \left(\frac{3(n-1)}{n}\right)^3 - 16.
\end{aligned}
$$

Let $g(x) = (\frac{x-1}{x-2})^3 + (\frac{3(x-1)}{x})^3 - 16$, where $x \geq 5$. We have

$$\begin{aligned} g'(x) &= \frac{3^4(x-1)^2}{x^4} - \frac{3(x-1)^2}{(x-2)^4} \\ &= \frac{3(x-1)^2}{x^4(x-2)^2}\left(\sqrt{27}(x-2)^2 + x^2\right) \\ &\quad \times \left(\sqrt[4]{27}(x-2) + x\right)\left(\sqrt[4]{27}(x-2) - x\right) \\ &> 0 \end{aligned}$$

for $x \geq 5$. Then $g(n) \geq g(5) = (\frac{4}{3})^3 + (\frac{12}{5})^3 - 16 > 0$. Therefore, this completes the proof of Theorem 4.4. □

Competing interests
The authors declare that they have no competing interests.

Authors' contributions
All authors completed the paper together. All authors read and approved the final manuscript.

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