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Bounds on Augmented Zagreb Index*

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Abstract

The augmented Zagreb index (AZI index) of a graph G, which is a valuable predictive index in the study of the heat of formation in octanes and heptanes, is defined as

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

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. As improvements and supplements for the previous results, in this paper, we obtain some bounds on the AZI indices of connected graphs by using different graph parameters, and characterize the corresponding extremal graphs.

1 Introduction

Let $G = (V(G),\ E(G))$ be a simple graph with vertex set $V(G)$ and edge set $E(G)$. Let $N(u)$ be the set of all neighbors of $u \in V(G)$, and d_u be the degree of u in G. A vertex u is called a pendent vertex if $d_u = 1$. Denote by Δ (resp. δ) the maximum (resp. minimum) degree of G. Let S_n and P_n denote the star and path of order n, respectively.

Molecular descriptors play a significant role in chemistry, pharmacology, etc. Among them, topological indices have a prominent place [5]. The augmented Zagreb index (AZI index for short) was firstly introduced by B. Furtula et al. in [2], which is defined to be

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

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It has been shown that AZI index is a valuable predictive index in the study of the heat of formation in octanes and heptanes [2], whose prediction power is better than atom-bond connectivity index (see [1, 3, 6]).

For the research of AZI index, B. Furtula et al. [2] firstly obtained some tight upper and lower bounds for the AZI index of a chemical tree, and determined the trees of order n with minimal AZI index. Moreover, Y. Huang et al. [4] gave some attained upper and lower bounds on the AZI index and characterized the corresponding extremal graphs.

As improvements and supplements for the results in [2, 4], in this paper, we obtain some bounds on the AZI indices of connected graphs by using different graph parameters, and characterize the corresponding extremal graphs.

2 Main results

For positive integers $i,\ j,\ \Delta$ with $i \leq j \leq \Delta$ and $\Delta \geq 3$, let

$$\begin{aligned} h(i,\ j,\ \Delta) &= \left(\frac{ij}{i+j-2}\right)^3 + 8\left(\frac{2}{i}+\frac{2}{j}-2-\frac{2}{\Delta}\right) - \left(\frac{\Delta}{\Delta-1}\right)^3\left(\frac{2}{i}+\frac{2}{j}-1-\frac{2}{\Delta}\right) \\ &= \left(\frac{ij}{i+j-2}\right)^3 - 8 + 2\left[8-\left(\frac{\Delta}{\Delta-1}\right)^3\right]\left(\frac{1}{i}+\frac{1}{j}-\frac{1}{2}-\frac{1}{\Delta}\right). \end{aligned}$$

Lemma 2.1 *Let $i,\ \Delta$ be positive integers with $3 \leq i \leq \Delta$. Then $h(i,\ i,\ \Delta) > 0$.*

Proof. Clearly, $h(i,\ i,\ \Delta) = \left(\frac{i^2}{2i-2}\right)^3 - 8 + 2\left[8-\left(\frac{\Delta}{\Delta-1}\right)^3\right]\left(\frac{2}{i}-\frac{1}{2}-\frac{1}{\Delta}\right)$ and

$$\frac{\partial(h(i,\ i,\ \Delta))}{\partial i} = \frac{2}{i^2}\left[\frac{i^7(3i-6)}{(2i-2)^4} + \frac{2\Delta^3}{(\Delta-1)^3} - 16\right].$$

Let $f(i) = \frac{i^7(3i-6)}{(2i-2)^4}$. Note that $\frac{d(f(i))}{di} = \frac{3i^6(2i^2-7i+7)}{8(i-1)^5} > 0$ since $i \geq 3$. Hence $f(i) \geq f(3)$ and then

$$\frac{\partial(h(i,\ i,\ \Delta))}{\partial i} \geq \frac{2}{i^2}\left[\frac{3^8}{4^4} + \frac{2\Delta^3}{(\Delta-1)^3} - 16\right] > 0.$$

It follows that $h(i,\ i,\ \Delta) \geq h(3,\ 3,\ \Delta)$. Obviously,

$$h(3,\ 3,\ \Delta) = \left(\frac{9}{4}\right)^3 - 8 + 2\left[8-\left(\frac{\Delta}{\Delta-1}\right)^3\right]\left(\frac{1}{6}-\frac{1}{\Delta}\right).$$

If $\Delta \geq 6$, since $\left(\frac{\Delta}{\Delta-1}\right)^3 < 8$ and $\frac{1}{6} \geq \frac{1}{\Delta}$, then $h(3,\ 3,\ \Delta) > 0$. If $\Delta = 3,\ 4,\ 5$, then

$$h(3,\ 3,\ 3) = \left(\frac{9}{4}\right)^3 - 8 + 2\left[8-\left(\frac{3}{2}\right)^3\right]\left(\frac{1}{6}-\frac{1}{3}\right) > 0,$$

$$h(3,\ 3,\ 4) = \left(\frac{9}{4}\right)^3 - 8 + 2\left[8 - \left(\frac{4}{3}\right)^3\right]\left(\frac{1}{6} - \frac{1}{4}\right) > 0,$$

$$h(3,\ 3,\ 5) = \left(\frac{9}{4}\right)^3 - 8 + 2\left[8 - \left(\frac{5}{4}\right)^3\right]\left(\frac{1}{6} - \frac{1}{5}\right) > 0.$$

Consequently, we obtain that $h(i,\ i,\ \Delta) > 0$ for $3 \leq i \leq \Delta$. □

Lemma 2.2 *Let $i,\ j,\ \Delta$ be positive integers with $i \leq j \leq \Delta$ and $\Delta \geq 3$. Then $h(i,\ j,\ \Delta) > 0$ for $(i,\ j) \neq (1,\ \Delta),\ (2,\ \Delta)$.*

Proof. Note that $(i,\ j) \neq (1,\ \Delta),\ (2,\ \Delta)$, then $j < \Delta$ if $i = 1,\ 2$. Clearly, $f(x) = \frac{x}{x-1}$ is decreasing for $x \geq 2$, and $f(2) = 2$. Since $j < \Delta$ if $i = 1,\ 2$, then $\frac{2}{j} > \frac{2}{\Delta}$, and it leads to

$$\begin{aligned} h(1,\ j,\ \Delta) &= \left(\frac{j}{j-1}\right)^3 - 8 + 2\left[8 - \left(\frac{\Delta}{\Delta-1}\right)^3\right]\left(\frac{1}{j} + \frac{1}{2} - \frac{1}{\Delta}\right) \\ &= \left(\frac{j}{j-1}\right)^3 - \left(\frac{\Delta}{\Delta-1}\right)^3 + \left[8 - \left(\frac{\Delta}{\Delta-1}\right)^3\right]\left(\frac{2}{j} - \frac{2}{\Delta}\right) > 0, \end{aligned}$$

and

$$h(2,\ j,\ \Delta) = \left[8 - \left(\frac{\Delta}{\Delta-1}\right)^3\right]\left(\frac{2}{j} - \frac{2}{\Delta}\right) > 0.$$

Now we may assume that $i \geq 3$, then $3 \leq i \leq j \leq \Delta$. Since the function $g(i,\ j) = \frac{j}{i+j-2}$ is increasing for $j\ (\geq i \geq 3)$, we have $g(i,\ j) \geq g(i,\ i)$ and then

$$\begin{aligned} \frac{\partial h(i,\ j,\ \Delta)}{\partial j} &= \frac{1}{j^2}\left[3i^3(i-2)\left(\frac{j}{i+j-2}\right)^4 + 2\left(\frac{\Delta}{\Delta-1}\right)^3 - 16\right] \\ &\geq \frac{1}{j^2}\left[3i^3(i-2)\left(\frac{i}{2i-2}\right)^4 + 2\left(\frac{\Delta}{\Delta-1}\right)^3 - 16\right]. \end{aligned}$$

Let $k(i) = 3i^3(i-2)\left(\frac{i}{2i-2}\right)^4$. Then for $i \geq 3$,

$$\frac{dk(i)}{di} = \frac{3i^6(2i^2 - 7i + 7)}{8(i-1)^5} > 0.$$

Hence $k(i) \geq k(3)$ and then

$$\frac{\partial h(i,\ j,\ \Delta)}{\partial j} \geq \frac{1}{j^2}\left[3^4 \cdot \left(\frac{3}{4}\right)^4 + 2\left(\frac{\Delta}{\Delta-1}\right)^3 - 16\right] > 0.$$

It follows that $h(i,\ j,\ \Delta) \geq h(i,\ i,\ \Delta)$ if $3 \leq i \leq j \leq \Delta$. Combining this with Lemma 2.1, we immediately get that $h(i,\ j,\ \Delta) \geq h(i,\ i,\ \Delta) > 0$ for $3 \leq i \leq j \leq \Delta$. □

Let G be a connected graph with $n \geq 3$ vertices and maximum degree Δ. Let n_i denote the number of vertices with degree i in G for $1 \leq i \leq \Delta$, and x_{ij} denote the number of edges of G

connecting vertices of degree i and j, where $1 \leq i \leq j \leq \Delta$. Let $A_{ij} = \frac{ij}{i+j-2}$, where $i,\ j$ are positive integers. Obviously, $x_{ij} = x_{ji}$ and $A_{ij} = A_{ji}$. Then the augmented Zagreb index of G can be rewritten as

$$AZI(G) = \sum_{\substack{1\leq i\leq j\leq\Delta \\ i+j\neq 2}} x_{ij}A_{ij}^3.$$

Let $\Psi_{n,\ m,\ \Delta}$ be the set of connected graphs with n vertices, m edges and maximum degree Δ each of whose edges has one end-vertex of degree Δ and the other end-vertex of degree 1 or 2.

Theorem 2.3 *Let G be a connected graph of order $n \geq 3$ with m edges and maximum degree Δ, where $2 \leq \Delta \leq n-1$. Then*

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

with equality if and only if $G \cong P_n$ for $\Delta = 2$, and $G \in \Psi_{n,\ m,\ \Delta}$ with $m \equiv 0\ (mod\ \Delta)$ for $\Delta \geq 3$.

Proof. If $\Delta = 2$, then $G \cong P_n$ and the result follows. Assume that $3 \leq \Delta \leq n-1$. Since G is a connected graph with n vertices, m edges and maximum degree Δ, then

$$\begin{cases} n_1 + n_2 + \cdots + n_\Delta = n, \\ n_1 + 2n_2 + \cdots + \Delta n_\Delta = 2m, \\ \sum_{2\leq i\leq\Delta} x_{1i} = n_1, \\ \sum_{1\leq j\leq\Delta,\ j\neq i} x_{ij} + 2x_{ii} = in_i \qquad (i = 2,\ 3,\ \ldots,\ \Delta). \end{cases}$$

Suppose that

$$\begin{cases} y_1 = \sum_{2\leq i\leq\Delta-1} x_{1i}, \\ y_2 = \sum_{1\leq j\leq\Delta-1, j\neq 2} x_{2j} + 2x_{22}, \\ y_i = \sum_{1\leq j\leq\Delta, j\neq i} x_{ij} + 2x_{ii} \qquad (i = 3,\ 4,\ \ldots,\ \Delta-1), \\ y_\Delta = \sum_{3\leq j\leq\Delta-1} x_{j\Delta} + 2x_{\Delta\Delta}, \end{cases}$$

i.e.,

$$\begin{cases} y_1 = n_1 - x_{1\Delta}, \\ y_2 = 2n_2 - x_{2\Delta}, \\ y_i = in_i \qquad (i = 3,\ 4,\ \ldots,\ \Delta-1), \\ y_\Delta = \Delta n_\Delta - x_{1\Delta} - x_{2\Delta}. \end{cases}$$

It follows that

$$\begin{cases} \sum_{1\leq i\leq\Delta} y_i = 2m - 2(x_{1\Delta} + x_{2\Delta}), \\ \sum_{1\leq i\leq\Delta} \frac{y_i}{i} = n - \left(1 + \frac{1}{\Delta}\right) x_{1\Delta} - \left(\frac{1}{2} + \frac{1}{\Delta}\right) x_{2\Delta}. \end{cases}$$

Then we get

$$x_{1\Delta} \quad = \quad \left(2n - m - \frac{2m}{\Delta}\right) - \sum_{1\leq i\leq\Delta} \left(\frac{2}{i} - \frac{1}{2} - \frac{1}{\Delta}\right) y_i$$

$$= \left(2n - m - \frac{2m}{\Delta}\right) - \sum_{\substack{1\le i\le j\le\Delta,\ i+j\ne 2\\ (i,\ j)\ne(1,\ \Delta),\ (2,\ \Delta)}} \left(\frac{2}{i} + \frac{2}{j} - 1 - \frac{2}{\Delta}\right) x_{ij},$$

and

$$\begin{aligned} x_{2\Delta} &= \left(2m + \frac{2m}{\Delta} - 2n\right) + \sum_{1\le i\le\Delta} \left(\frac{2}{i} - 1 - \frac{1}{\Delta}\right) y_i \\ &= \left(2m + \frac{2m}{\Delta} - 2n\right) + \sum_{\substack{1\le i\le j\le\Delta,\ i+j\ne 2\\ (i,\ j)\ne(1,\ \Delta),\ (2,\ \Delta)}} \left(\frac{2}{i} + \frac{2}{j} - 2 - \frac{2}{\Delta}\right) x_{ij}. \end{aligned}$$

Consequently, by Lemma 2.2, we obtain that

$$\begin{aligned} AZI(G) &= \left(\frac{\Delta}{\Delta-1}\right)^3 x_{1\Delta} + 8x_{2\Delta} + \sum_{\substack{1\le i\le j\le\Delta,\ i+j\ne 2\\ (i,\ j)\ne(1,\ \Delta),\ (2,\ \Delta)}} \left(\frac{ij}{i+j-2}\right)^3 x_{ij} \\ &= \left(\frac{\Delta}{\Delta-1}\right)^3 \left(2n - m - \frac{2m}{\Delta}\right) + 8\left(2m + \frac{2m}{\Delta} - 2n\right) + \sum_{\substack{1\le i\le j\le\Delta,\ i+j\ne 2\\ (i,\ j)\ne(1,\ \Delta),\ (2,\ \Delta)}} h(i,\ j,\ \Delta) x_{ij} \\ &\ge \left(\frac{\Delta}{\Delta-1}\right)^3 \left(2n - m - \frac{2m}{\Delta}\right) + 8\left(2m + \frac{2m}{\Delta} - 2n\right) \end{aligned}$$

with equality if and only if $x_{ij} = 0$ for $1 \le i \le j \le \Delta,\ i + j \ne 2,\ (i,\ j) \ne (1,\ \Delta),\ (2,\ \Delta)$, implying that

$$\begin{cases} x_{1\Delta} = 2n - m - \frac{2m}{\Delta}, \\ x_{2\Delta} = 2m + \frac{2m}{\Delta} - 2n, \end{cases}$$

that is, $G \in \Psi_{n,\ m,\ \Delta}$ with $m \equiv 0\ (mod\ \Delta)$ for $\Delta \ge 3$. □

Lemma 2.4 *([4]) Let G be a connected graph with* $m \ge 2$ *edges and maximum degree* $\Delta \ge 2$. *Then*

$$AZI(G) \ge \frac{m\Delta^3}{(\Delta-1)^3}$$

with equality if and only if $G \cong S_{m+1}$.

Remark 1 *Since* $\left(\frac{\Delta}{\Delta-1}\right)^3 \le 8\ (\Delta \ge 2)$ *and* $n \le m + 1 \le m + \frac{m}{\Delta}$ *for a connected graph G, then*

$$\left(\frac{\Delta}{\Delta-1}\right)^3 \left(2n - m - \frac{2m}{\Delta}\right) + 8\left(2m + \frac{2m}{\Delta} - 2n\right) - \frac{m\Delta^3}{(\Delta-1)^3} = \left[\left(\frac{\Delta}{\Delta-1}\right)^3 - 8\right]\left(2n - 2m - \frac{2m}{\Delta}\right) \ge 0.$$

Hence the lower bound for the AZI index of a connected G given in Theorem 2.3 is an improvement of that in Lemma 2.4 ([4]).

For $3 \le \Delta \le n - 2$ and $n \equiv 1\ (mod\ \Delta)$, let $\mathcal{T}_{n,\ \Delta}$ be the set of trees obtained by subdividing every edge of a tree on $\frac{n-1}{\Delta}$ vertices with maximum degree at most Δ, whose vertices are denoted by $v_1,\ v_2,\ \dots,\ v_{\frac{n-1}{\Delta}}$, and then attaching some pendent vertices to v_i until the degree of v_i is equal to Δ for $i = 1,\ 2,\ \dots,\ \frac{n-1}{\Delta}$. Let $\mathcal{T}_{n,\ n-1} = \{S_n\}$. It can be seen that $\mathcal{T}_{n,\ \Delta} = \Psi_{n,\ n-1,\ \Delta}$ with $n - 1 \equiv 0\ (mod\ \Delta)$ for $3 \le \Delta \le n - 1$. By Theorem 2.3, we have

Corollary 2.5 *Let T be a tree with n vertices and maximum degree Δ, where $n \geq 3$ and $2 \leq \Delta \leq n-1$. Then*

$$AZI(T) \geq \left(\frac{\Delta}{\Delta-1}\right)^3 \left[n+1-\frac{2(n-1)}{\Delta}\right] + 8\left[\frac{2(n-1)}{\Delta}-2\right]$$

with equality if and only if $T \cong P_n$ for $\Delta = 2$, and $T \in \mathcal{T}_{n,\Delta}$ with $n \equiv 1\ (mod\ \Delta)$ for $\Delta \geq 3$.

A tree is called a chemical tree if $\Delta \leq 4$. Note that if $2 \leq \Delta \leq 4$, then

$$\begin{aligned}
& \left(\frac{\Delta}{\Delta-1}\right)^3 \left[n+1-\frac{2(n-1)}{\Delta}\right] + 8\left[\frac{2(n-1)}{\Delta}-2\right] \\
= \ & \left[8-\left(\frac{\Delta}{\Delta-1}\right)^3\right]\left[\frac{2(n-1)}{\Delta}-n-1\right] + 8(n-1) \\
\geq \ & \left[8-\left(\frac{4}{3}\right)^3\right]\left[\frac{n-1}{2}-n-1\right] + 8(n-1) \\
= \ & \frac{140n}{27}-\frac{148}{9},
\end{aligned}$$

and it follows from Corollary 2.5 that

Corollary 2.6 *([2]) Let T be a chemical tree with n vertices, where $n \geq 3$. Then*

$$AZI(T) \geq \frac{140n}{27}-\frac{148}{9}$$

with equality if and only if $T \in \mathcal{T}_{n,4}$ with $n \equiv 1\ (mod\ 4)$.

Remark 2 *In [2], the authors only obtained the lower bound for the AZI index of a chemical tree, but did not characterize the corresponding extremal chemical trees.*

Lemma 2.7 *([4])* (1) *A_{1j} is decreasing for $j \geq 2$.*

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

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

A graph in which every vertex has the same degree is regular. A graph is biregular if it has unequal maximum and minimum degrees and every vertex has one of those two degrees.

Let Φ_1 be the class of connected graphs whose pendent vertices are adjacent to the maximum degree vertices and all other edges have at least one end-vertex of degree 2. Let Φ_2 be the class of connected graphs whose vertices are of degree at least two and all the edges have at least one end-vertex of degree 2.

Theorem 2.8 *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*

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

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 $G \in \Phi_2$.

Proof. Since G is a connected graph of order n with m edges, p pendent vertices, maximum degree Δ and minimum non-pendent vertex degree δ_1, we have the following two cases.

Case 1. $\delta_1 = 2$. It follows from Lemma 2.7 that

$$\begin{aligned} AZI(G) &= \sum_{2\leq j\leq \Delta} x_{1j}A_{1j}^3 + \sum_{2\leq i\leq j\leq \Delta} x_{ij}A_{ij}^3 \\ &\geq pA_{1\Delta}^3 + \sum_{2\leq i\leq j\leq \Delta} x_{ij}A_{2j}^3 \\ &= p\left(\frac{\Delta}{\Delta-1}\right)^3 + 8(m-p), \end{aligned}$$

with equality if and only if G is a $(1,\ \Delta)$-biregular graph or $G \in \Phi_1$ or $G \in \Phi_2$.

Case 2. $\delta_1 > 2$. By Lemma 2.7, we have

$$\begin{aligned} AZI(G) &\geq pA_{1\Delta}^3 + (m-p)A_{\delta_1,\ \delta_1}^3 \\ &= p\left(\frac{\Delta}{\Delta-1}\right)^3 + (m-p)\left(\frac{\delta_1^2}{2\delta_1-2}\right)^3, \end{aligned}$$

with equality if and only if $x_{ij} = 0$ for $1 \leq i \leq j \leq \Delta$ but $(i,\ j) \neq (1,\ \Delta)$ and $(\delta_1,\ \delta_1)$, that is, G is isomorphic to a $(1,\ \Delta)$-biregular graph or a regular graph. □

Let Φ_3 be the set of trees whose pendent vertices are adjacent to the maximum degree vertices and all other edges have at least one end-vertex of degree 2. By Theorem 2.8, we have the following corollary.

Corollary 2.9 *Let T be a tree of order $n \geq 3$ with p pendent vertices, maximum degree Δ and minimum non-pendent vertex degree δ_1. Then*

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

with equality if and only if T is isomorphic to a $(1,\ \Delta)$-biregular tree or $T \in \Phi_3$.

Theorem 2.10 *Let G be a connected graph of order n with m edges, p pendent vertices, maximum degree* Δ *and minimum non-pendent vertex degree* δ_1. *Then*

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

with equality if and only if G is a regular graph or G is a $(1,\ \delta_1)$*-biregular graph.*

Proof. Since G is a connected graph of order n with m edges, p pendent vertices, maximum degree Δ and minimum non-pendent vertex degree δ_1, by Lemma 2.7, then

$$\begin{aligned} AZI(G) &\leq pA^3_{1,\ \delta_1} + (m-p)A^3_{\Delta,\ \Delta} \\ &= p\left(\frac{\delta_1}{\delta_1 - 1}\right)^3 + (m-p)\left(\frac{\Delta^2}{2\Delta - 2}\right)^3. \end{aligned}$$

The equality holds if and only if G is a regular graph or G is a $(1,\ \delta_1)$-biregular graph. □

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