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Further Results on the Augmented Zagreb Index

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Abstract: **The augmented Zagreb index of a simple connected graph G is defined as $\sum_{uv\in E(G)}(\frac{d_u d_v}{d_u+d_v-2})^3$, where d_u is the degree of vertex u in G. A connected graph G is called a quasi-tree graph if there exists a vertex $u_0\in V(G)$ such that $G-u_0$ is a tree. A connected graph G is a cactus if any two of its cycles have at most one common vertex. In this paper, we determine the smallest and the second-smallest *AZI* indices of quasi-tree graphs and the minimal *AZI* index in the class of all cacti graphs with n vertices and r cycles.**

Keywords: **Augmented Zagreb index, Quasi-tree, Cactus, Extremal graph.**

I. INTRODUCTION

Let G be a simple, finite and undirected graph with vertex set $V(G)$ and edge set $E(G)$. For $v\in V(G)$, the degree of v, denoted by d_v, is the number of edges incident to v. A vertex u is called a pendent vertex if $d_u=1$. If u and v are two adjacent vertices of G, then the edge connecting them will be denoted by uv. A description of the structure of 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 have a prominent place [28]. Inspired by the ABC index [5-7], Furtula et al. [1] introduce a new topological index called augmented Zagreb index (AZI index for short) defined as

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

Boris Furtula et al. [1] proved that AZI is a valuable predictive index in the study of the heat of formation in heptanes and octanes, whose prediction power is better than atom-bond connectivity index. Moreover, Gutman and Tošovič [2] tested the correlation abilities of 20 vertex-based topological indices for the case of standard heats of formation and normal boiling points of octane isomers, and they found that the AZI index yield the best results.

Let G be a simple graph. The neighborhood of a vertex $u\in V(G)$ will be denoted by $N_G(u)$. $\Delta(G)=max\{d_u \mid u\in V(G)\}$ and $\delta(G)=min\{d_u \mid u\in V(G)\}$. If $W\subset V(G)$, we denote by $G-W$ the subgraph of G obtained by deleting the vertices of W and the edges incident with them. Similarly, if $E\subset E(G)$, we denote by $G-E$ the subgraph of G obtained by deleting the edges of E. If $W=\{v\}$ and $E=\{xy\}$, we write $G-v$ and $G-xy$ instead of $G-\{v\}$ and $G-\{xy\}$, respectively. As usual, C_n denotes the cycles on n vertices, S_n denotes the star on n vertices.

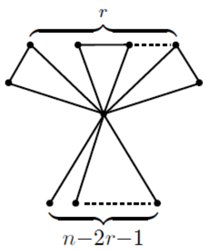

Figure 1.1 Graph $G(n,r)$

A connected graph G is called a quasi-tree if there exists $u \in V(G)$ such that $G-u$ is a tree. The concept of quasi-tree graph was first introduced in [23, 24]. Clearly any tree is a quasi-tree graph since the deletion of any pendent vertex will deduce another new tree. We call any tree a trivial quasi-tree graph, and other quasi-tree graphs are called non-trivial quasi-tree graphs. For convenience, let $Q(n)$ be the set of non-trivial quasi-tree graphs of order n. We call G a cactus if it is connected and all of blocks of G are either edges or cycles, i.e., any two of its cycles have at most one common vertex. Denote $G_{n,r}$ the set of cacti of order n and with r cycles. Let $G(n,r)$ denote the cactus obtained by adding r independent edges to the star S_n (see Figure 1.1). Note that $G(n,r) \in G_{n,r}$.

Furtula et al. [1] obtained upper and lower bounds of the AZI index of a chemical tree and showed that among all trees, the star graph has the minimum AZI value. Y. Huang et al. [8] and D. Wang et al. [9] provided particular bounds on the AZI indices of connected graphs and characterized the corresponding extremal graphs. A. Ali et al. [3] established inequalities between AZI and several other vertex-degree-based topological indices. A. Ali et al. [4] 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 light of the information available for AZI of trees, unicyclic graphs, bicyclic graphs, et al., it is natural to consider other classes of graphs, the quasi-tree graphs and the cactus graph are a reasonable starting point for such an investigation. For results on the topological indices of quasi-tree graphs, one may refer to [25-27]. On the other hand, cacti represent important class of molecules [13-17] and has been reported in mathematical literature [10,11,21,22]. In this paper, we give the smallest and the second-smallest AZI indices of quasi-tree graphs. Moreover, we determine graphs with the minimal AZI index among all the cacti with n vertices and r cycles.

Now, we give the following lemmas that will be used in the proof of our main results. For convenience, let $A(x,y) = (\frac{xy}{x+y-2})^3$ for $x, y \geq 1$ and $x+y>2$. Obviously, $A(x,y) = A(y,x)$.

Lemma 1.1 ([7]) (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 1.2 ([7]) $A(1,\Delta) \leq A(1,i) \leq A(1,2) = A(2,j) < A(3,3) \leq A(k,l) \leq A(\Delta,\Delta)$, where $2 \leq i, j \leq \Delta$ and $3 \leq k \leq l \leq \Delta$.

Lemma 1.3 ([7]) Let G be a connected graph of order $n \geq 3$, and $G \ncong K_n$. Then $AZI(G) < AZI(G+e)$, where $e \notin E(G)$.

II. THE AZI INDEX OF QUASI-TREE GRAPHS

In this section, we shall give the smallest and the second-smallest AZI indices of quasi-tree graphs. The corresponding extremal graphs are characterized.

Theorem 2.1 Let $G \in Q(n)$ with $n \geq 3$, then

$$AZI(G) \geq (n-3)(\frac{n-1}{n-2})^3 + 24$$

with equality if and only if $G \cong G(n,1)$.

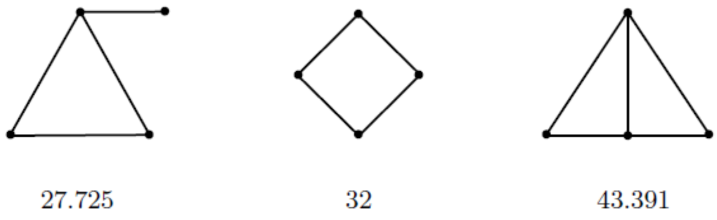

Figure 2.2 $AZI(G)$ **of** $\mathrm{Q}(4)$

Proof: We proof this result by induction on n. When $n=3$, there is only one non-trivial quasi-tree graph C_3, then the result holds. If $n=4$, there are only three graphs in $\mathrm{Q}(n)$ (see Figure 2.2), then theorem holds clearly. In the following we assume that $n \geq 5$ and the result holds for all quasi-tree graphs in $\mathrm{Q}(n-1)$. We choose $G \in \mathrm{Q}(n)$ such that $AZI(G)$ is as small as possible.

First, we establish the following claim.

Claim 1: There exists at least one pendent vertex in G.

Suppose that $\delta(G) \geq 2$. By Lemma 1.2 and some elementary calculation, we conclude that $AZI(C_n) = 8n > (n-3)A(1,n-1)+24$. Thus $G \ncong C_n$. So G contains at least two cycles. Assume that there is any edge $e = xy$ of a cycle in G. Note that $G-e \in \mathrm{Q}(n)$. Let $N_G(x) \setminus \{y\} = \{x_1, x_2, \ldots, x_{d_x-1}\}$ and $N_G(y) \setminus \{x\} = \{y_1, y_2, \ldots, y_{d_y-1}\}$. By Lemma 1.1, we have

$$\begin{aligned} AZI(G) = AZI(G-e) + A(d_x, d_y) + \sum_{i=1}^{d_x-1}\big(A(d_x, d_{x_i}) - A(d_x - 1, d_{x_i})\big) \\ + \sum_{i=1}^{d_y-1}\big(A(d_y, d_{y_i}) - A(d_y - 1, d_{y_i})\big) \\ > AZI(G-e). \end{aligned}$$

This is a contradiction to the choice of G. This completes the Claim 1.

By Claim 1, we may assume that there is a pendent vertex u in G adjacent to a vertex v. If $d_v = d$, then $2 \leq d \leq n-1$. Denote $N_G(v) \setminus \{u\} = \{v_1, v_2, \ldots, v_{d-1}\}$, $d_{v_1} = d_{v_2} = \cdots = d_{v_{k-1}} = 1$ and $d_{v_j} \geq 2$, for $k \leq j \leq d-1$, where $k \geq 1$. Let $G' = G - u - v_1 - v_2 - \cdots - v_{k-1}$. Note that $G' \in \mathrm{Q}(n-k)$. By induction hypothesis and Lemma 1.2, we have

$$\begin{aligned} AZI(G) &= AZI(G') + kA(1,d) + \sum_{i=k-1}^{d-1}\big(A(d, d_{v_i}) - A(d-k, d_{v_i})\big) \\ &\geq (n-k-3)A(1, n-k-1) + 24 + kA(1,d) + \sum_{i=k-1}^{d-1}\big(A(d, d_{v_i}) - A(d-k, d_{v_i})\big) \\ &\geq (n-k-3)A(1, n-k-1) + kA(1,d) + 24 \\ &= (n-3)A(1,n-1) + 24 + (n-k-3)\big(A(1,n-k-1) - A(1,n-1)\big) + k\big(A(1,d) - A(1,n-1)\big) \\ &\geq (n-3)A(1,n-1) + 24. \end{aligned}$$

The above equality holds if and only if $k = n-3$, $d = n-1$, $d_{v_i} = 2$ for $1 \leq i \leq d-1$ and $G' \cong G(n-k,1)$. Therefore $G \cong G(n,1)$, which completes the proof of this theorem.

Let $Q_{n,4}$ be an n-vertex graph obtained from C_4 by attaching $n-4$ pendant edges to one vertex of C_4.

Theorem 2.2: Let $G \in \mathrm{Q}(n)$ with $n \geq 4$ and $G \not\cong G(n,1)$. Then

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

with equality if and only if $G \cong Q_{n,4}$.

Proof: By induction on n. If $n=4$, then the theorem holds clearly (see Figure 2.2). In Figure 2.3, all 5-vertex non-trivial quasi-tree graphs are drawn. From this figure, one can prove graph $Q_{4,3}$ has the second-smallest AZI index in $\mathrm{Q}(n)$. Assume that $G \in \mathrm{Q}(n) \setminus \{Q_{n,4}\} (n > 5)$ has the minimum AZI index among all members of $\mathrm{Q}(n) \setminus \{Q_{n,4}\}$. Using a similar reasoning as that in the proof of Theorem 2.1, we find that $\delta(G) = 1$.

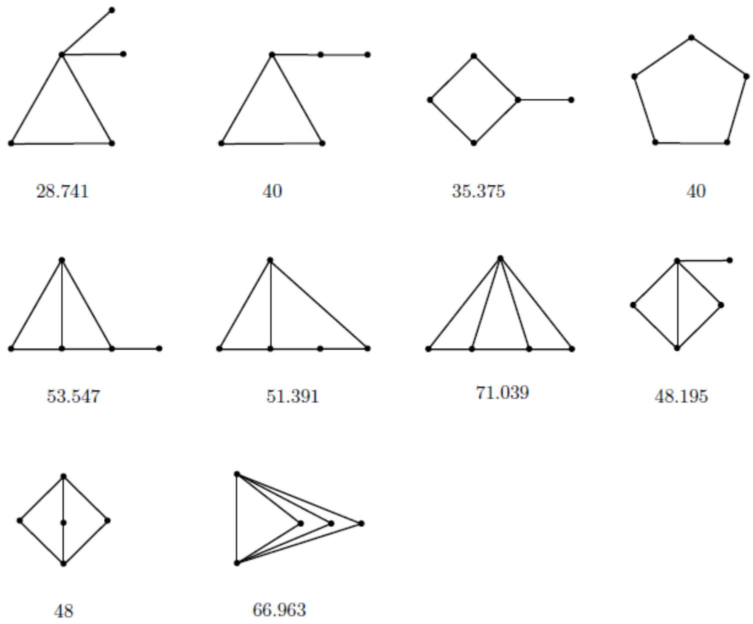

Figure 2.3 $AZI(G)$ **of** $\mathrm{Q}(5)$

Let u be pendant vertex and v be the neighbor of u. Denote $d_v = d$. We might distinguish two cases to obtain our result.

Case 1: $d = n-1$.

First we define an quasi-tree graph $Q'(n)$ by connecting one pendant vertices and one vertex of degree two of $G(n,1)$. By Lemma 1.3, one can see that $AZI(Q'(n)) > AZI(G(n,1))$. By Lemma 1.2 we have $(n-4)A(1,n-2) - (n-4)A(1,n-1) - A(3,n-1) < 0$, then $AZI(Q_{n,4}) < AZI(Q'(n))$. Thus, $AZI(G) > AZI(Q_{n,4})$.

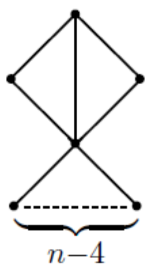

Figure 2.4 Graphs of $Q'(n)$

Case 2: $2 \le d \le n-2$.

Denote $N_G(v) \setminus \{u\} = \{y_1, y_2, \ldots, y_{d-1}\}$. Assume, without loss generality, that $d(y_1) = d(y_2) == d(y_{k-1}) = 1$ and $d(y_i) \ge 2$ for $k \le i \le d-1$, where $k \ge 1$. Let $G' = G - u - y_1 - y_2 - \cdots - y_{k-1}$. Note that $G' \in \mathrm{Q}(n-k)$. By induction hypothesis and Lemma 1.1, we have

$$AZI(G) = AZI(G') + kA(1,d) + \sum_{i=k}^{d-1}\Big(A(d, d_{y_i}) - A(d-1, d_{y_i})\Big)$$

$$\ge (n-k-4)A(1, n-k-2) + 32 + kA(1,d) + \sum_{i=k}^{d-1}\Big(A(d, d_{y_i}) - A(d-1, d_{y_i})\Big)$$

$$\ge (n-k-4)A(1, n-k-2) + kA(1,d) + 32$$

$$= (n-4)A(1, n-2) + 32 + (n-k-4)\Big(A(1, n-k-2) - A(1, n-2)\Big)$$

$$+k\Big(A(1,d) - A(1, n-2)\Big)$$

$$\ge (n-4)A(1, n-2) + 32.$$

The above equality holds if and only if $k = n-4$, $d = n-2$, $d_{y_i} = 2$ for $k \le i \le d-1$ and $G' \cong Q_{n-k-4,4}$. Therefore $G \cong Q_{n,4}$, which completes the proof of this theorem.

III. THE *AZI* INDEX OF CACTI GRAPHS

It is clearly that $\mathrm{G}_{n,0}$ is the set of trees of order n and $\mathrm{G}_{n,1}$ is the set of unicyclic graphs of order n. Furtula et al. [1] proved that the star graph has the minimal AZI value among all trees.

Lemma 3.1: ([1]) Let $G \in \mathrm{G}_{n,0}$ and $n \ge 2$, then

$$AZI(G) \ge \frac{(n-1)^4}{(n-2)^3}$$

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

F. Zhan et al. [12] gave the lower bound for the AZI index of unicyclic graphs and characterized extremal graph.

Lemma 3.2: ([12]) Let $G \in \mathrm{G}_{n,1}$ and $n \ge 3$, then

$$AZI(G) \ge (n-3)\Big(\frac{n-1}{n-2}\Big)^3 + 24$$

with equality if and only if $G \cong G(n,1)$.

Theorem 3.3: Let $G \in \mathrm{G}_{n,r}$, $n \ge 5$, then

$$AZI(G) \ge (n-2r-1)\Big(\frac{n-1}{n-2}\Big)^3 + 24r$$

with equality if and only if $G \cong G(n,r)$.

Proof: By induction on $n+r$. Let $\varphi(n,r) = (n-2r-1)\Big(\frac{n-1}{n-2}\Big)^3 + 24r$. If $r=0$ or $r=1$, then the theorem holds clearly by Lemma 3.1 and Lemma 3.2. Now we assume that $r \ge 2$ and $n = 5$. If $n = 5$, then the theorem holds clearly by the facts that there is only one graph in $\mathrm{G}_{5,2}$.

Let $G \in \mathcal{G}_{n,r}$, $n \geq 6$ and $r \geq 2$. We consider the following two cases.

Case 1: $\delta(G) = 1$.

Let $u \in V(G)$ with $d_u = 1$ and $uv \in E(G)$. If $d_v = d$, then $2 \leq d \leq n-1$. Let $N_G(v) \setminus \{u\} = \{x_1, x_2, ..., x_{d-1}\}$, $d_{x_1} = d_{x_2} = \cdots = d_{x_{k-1}} = 1$ and $d_{x_j} \geq 2$ for $k \leq j \leq d-1$, where $k \geq 1$.

Let $G' = G - u - x_1 - x_2 - \cdots - x_{k-1} \in \mathcal{G}_{n-k,r}$. By induction assumption and Lemma 1.1, we have

$$\begin{aligned} AZI(G) &= AZI(G') + kA(1,d) + \sum_{i=k-1}^{d-1} \left(A(d,d_{x_i}) - A(d-k,d_{x_i})\right) \\ &\geq \varphi(n-k,r) + kA(1,d) + \sum_{i=k-1}^{d-1} \left(A(d,d_{x_i}) - A(d-k,d_{x_i})\right) \\ &\geq \varphi(n-k,r) + kA(1,d) \\ &= \varphi(n,r) + (n-2r-k-1)\left(A(1,n-k-1) - A(1,n-1)\right) + k\left(A(1,d) - A(1,n-1)\right) \\ &\geq \varphi(n,r). \end{aligned}$$

The equality $AZI(G) = \varphi(n,r)$ holds if and only if equalities hold throughout the above inequalities, that is, if and only if $2r = n-k-1$, $d = n-1$ and $G' \cong G(n-k,r)$. So, $AZI(G) \geq \varphi(n,r)$ with equality if and only if $G \cong G(n,r)$.

Case 2: $\delta(G) \geq 2$.

In this case, by the definition of cactus, there exist two edges v_0v_1, $v_1v_2 \in E(G)$ such that $d_{v_1} = d_{v_2} = 2$ and $d_{v_0} = d \geq 3$. We will finish the proof by considering two subcases.

Subcase 2.1: $v_0v_2 \notin E(G)$.

Let $G' = G - v_1 + v_0v_2 \in \mathcal{G}_{n-1,r}$. Then

$$\begin{aligned} AZI(G) &= AZI(G') + A(2,d) + A(2,2) \\ &\geq \varphi(n-1,r) + A(2,d) + A(2,2) \\ &= \varphi(n,r) + (n-2r-2)\left(A(1,n-2) - A(1,n-1)\right) + 16 - A(1,n-1) \\ &> \varphi(n,r). \end{aligned}$$

Subcase 2.2: $v_0v_2 \in E(G)$.

Let $G' = G - v_1 - v_2 \in \mathcal{G}_{n-2,r-1}$ and $N_G(v_0) \setminus \{v_1, v_2\} = \{x_1, x_2, ..., x_{d-2}\}$. Then

$$\begin{aligned} AZI(G) &= AZI(G') + 2A(2,d) + A(2,2) + \sum_{i=1}^{d-2} \left(A(d_1,d_{x_i}) - A(d-2,d_{x_i})\right) \\ &\geq \varphi(n-2,r-1) + \sum_{i=1}^{d-2} \left(A(d,d_{x_i}) - A(d-2,d_{x_i})\right) + 24 \\ &\geq \varphi(n-2,r-1) + 24 \\ &= \varphi(n,r) + (n-2r-1)\left(A(1,n-3) - A(1,n-1)\right) \\ &\geq \varphi(n,r). \end{aligned}$$

The equality $AZI(G) = \varphi(n,r)$ holds if and only if equalities hold throughout the above inequalities, that is, if and only if $2r = n-1$ and $G' \cong G(n-2,r-1)$. Thus, we have $AZI(G) \geq \varphi(n,r)$ with equality if and only if $G \cong \varphi(n,r)$.

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