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A Note on Minimal Augmented Zagreb Index of Tricyclic Graphs of Fixed Order

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Abstract

Let G be a graph containing no component isomorphic to the path graph of order 2. Denote by d_u the degree of an arbitrary vertex u of G. The augmented Zagreb index (AZI) of G is the sum of the weights $(d_u\,d_v/(d_u+d_v-2))^3$ over all edges uv of G. In this note, the unique graph with minimal AZI is characterized from the class of all connected tricyclic graphs of order n for every $n \geq 6$, where a connected tricyclic graph of order n is a connected graph of order n and size $n+2$ with $n \geq 4$. The obtained result gives a partial solution to a problem posed in the recent paper [W. Lin, D. Dimitrov, R. Škrekovski, Complete characterization of trees with maximal augmented Zagreb index, *MATCH Commun. Math. Comput. Chem.* **83** (2020) 167–178].

1 Introduction and statement of the main result

All the graphs discussed in this note are finite, and they contain neither any loop nor multiple edges. The *vertex set* and *edge set* of a graph G are denoted by $V(G)$ and $E(G)$, respectively. The *degree* of a vertex $u \in V(G)$ is denoted by d_u. The edge of G, connecting the vertices u and v is denoted by uv. An *n-vertex graph* is a graph of order n. The minimum number of edges of a graph G whose removal makes G acyclic (graph containing no cycle) is its *cyclomatic number.* If t is a positive integer then by a *t-cyclic graph*, we mean a graph with cyclomatic number t. We call 1-cyclic, 2-cyclic and 3-cyclic graphs as *unicyclic*, *bicyclic* and *tricyclic graphs*, respectively. (It needs to be mentioned here that according to some authors, unicyclic, bicyclic and tricyclic graphs are always connected but according to some other authors (see for example [6,19]) and to our stated definition of these graphs, such graphs may or may not be connected.) The (chemical) graph theoretical notation and terminology that are not defined in this note can be found in some standard relevant textbooks, like [4, 5, 12, 20].

A *graph invariant* I is a numerical quantity associated with a graph G satisfying the equation $I(G) = I(G')$ for every graph G' isomorphic to G. The graph invariants that found some applications in chemistry are usually known as the *topological indices.* The *augmented Zagreb index* (AZI), introduced by Furtula *et al.* [8], is one of the graph invariants that have found considerable chemical applications – see for example the references [8, 9, 11, 13, 17] for the chemical applicability of AZI. For a graph G containing no component isomorphic to the 2-vertex path graph, this topological index is defined as

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

Because of the several chemical applications of AZI, its mathematical properties have been studied extensively in many papers, see for example some recent ones [7,10,15,16,18], recent review [3] (where the extremal results and bounds concerning this index have been summarized) and relevant references listed therein.

Furtula *et al.* [8] proved that the start graph S_n is the unique graph with minimal AZI among all n-vertex trees for every n greater than 3. In the papers [14, 21], it was shown independently that the graph obtained from S_n by adding one edge or two nonadjacent edges is the only graph having minimal AZI in the class of all n-vertex connected unicyclic or bicyclic graphs, respectively, for every n greater than 5. Recently, Lin *et al.* [16] posed a problem of finding graph(s) having minimal AZI among all n-vertex graphs of size m for $m \geq n + 2$. The main purpose of the present note is to solve the aforementioned problem of Lin *et al.* for the n-vertex connected tricyclic graphs (that are actually the n-vertex connected graphs of size $n + 2$) when $n \geq 6$.

Note that most of the topological indices for which star S_n has maximal/minimal values in the class of all n-vertex trees, their maximal/minimal values in the class of all n-vertex connected unicyclic/bicyclic/tricyclic graphs are usually attained by the graph(s) that can be deduced from S_n by adding one/two/three edge(s), respectively, in some specific way. Thus, at first sight, it was guessed that the graph with minimal AZI among all n-vertex connected tricyclic graphs would be the graph deduced from S_n by adding three edges in some specific way, but surprisingly that guess was wrong as it can be seen from the following main result of this note.

Theorem 1. *If n is a fixed integer greater than 5 then G_n^* is the unique graph with minimal AZI among all n-vertex connected tricyclic graphs, where the graph G_n^* is depicted in Figure 1.*

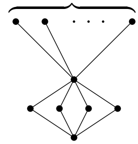

Figure 1. The n-vertex graph G_n^* where $n \geq 6$.

The following corollary is an immediate consequence of Theorem 1.

Corollary 1. *For $n \geq 6$, if G is an n-vertex connected tricyclic graph then*

$$AZI(G) \geq (n-6)\left(\frac{n-2}{n-3}\right)^3 + 64,$$

with equality if and only if G is isomorphic to the graph G_n^* shown in Figure 1.

2 Proof of Theorem 1

In order to prove Theorem 1, we firstly prove some lemmas.

Lemma 2. *If G is a graph of size m and minimum degree at least 2 such that it does not contain any component isomorphic to the 2-vertex path graph, then*

$$AZI(G) \geq 8m\,,$$

with equality if and only if at least one end-vertex of every edge of G has degree 2.

Proof. For $x \geq 2$ and $y \geq 2$, note that the function f defined by $f(x,y) = (xy/x+y-2)^3$, is increasing in both x and y in the interval $[2,\infty)$. Clearly, if x and y are integers greater than 1 then the output value of f is equal to $f(2,2)$ if and only if at least one of x and y is 2. Now, the desired result follows from the definition of AZI. ■

Lemma 3. *For $n \geq 6$, if G is an n-vertex connected tricyclic graph of minimum degree at least 2 then*

$$AZI(G) \geq (n-6)\left(\frac{n-2}{n-3}\right)^3 + 64,$$

with equality if and only if G is isomorphic to the graph G_n^* depicted in Figure 1.

Proof. Firstly, we assume that $n > 6$. Since the size of G is $n+2$, from Lemma 2 it follows that

$$AZI(G) \geq 8(n+2)\,. \tag{1}$$

Since $n > 6$, it holds that

$$(n-6)\left(8 - \left(\frac{n-2}{n-3}\right)^3\right) > 0\,,$$

which is equivalent to

$$8(n+2) > (n-6)\left(\frac{n-2}{n-3}\right)^3 + 64\,,$$

and hence from (1) it follows that

$$AZI(G) > (n-6)\left(\frac{n-2}{n-3}\right)^3 + 64.$$

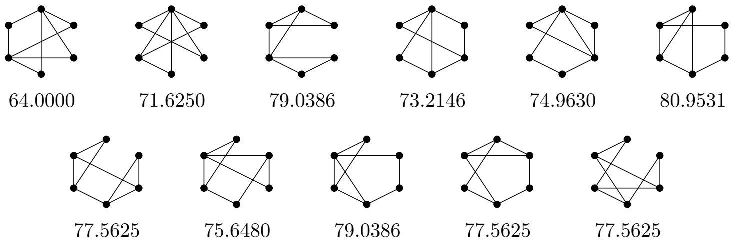

Figure 2. All non-isomorphic 6-vertex connected tricyclic graphs of minimum degree at least 2 together with their approximated AZI.

This completes the proof when $n > 6$. The required result, for the case $n = 6$, follows from Figure 2 where all the non-isomorphic 6-vertex connected tricyclic graphs of minimum degree at least 2, together with their approximated AZI, are depicted.

■

Lemma 4. *For $n \geq 6$, if G is an n-vertex connected tricyclic graph of maximum degree $n-1$ then*

$$AZI(G) > (n-6)\left(\frac{n-2}{n-3}\right)^3 + 64.$$

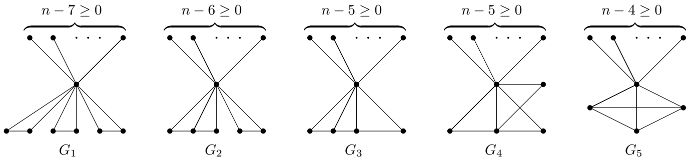

Figure 3. All possible non-isomorphic connected tricyclic graphs of order n and maximum degree $n-1$, where $n \geq 6$ (this figure is taken from [1]). Note that G_1 exists if and only if $n \geq 7$.

Proof. For $n \geq 6$, note that the graphs $G_1, G_2, \cdots, G_5$ depicted in Figure 3 are the only possible non-isomorphic connected tricyclic graphs of order n and maximum degree $n-1$. Simple calculations yield

$$AZI(G_1) = (n-7)\left(\frac{n-1}{n-2}\right)^3 + 72, \quad (\text{if } n \geq 7)$$

$$AZI(G_2) = (n-6)\left(\frac{n-1}{n-2}\right)^3 + 27\left(\frac{n-1}{n}\right)^3 + 56,$$

$$AZI(G_3) = (n-5)\left(\frac{n-1}{n-2}\right)^3 + 54\left(\frac{n-1}{n}\right)^3 + \frac{2777}{64},$$

$$AZI(G_4) = (n-5)\left(\frac{n-1}{n-2}\right)^3 + 64\left(\frac{n-1}{n+1}\right)^3 + 48,$$

and

$$AZI(G_5) = (n-4)\left(\frac{n-1}{n-2}\right)^3 + 81\left(\frac{n-1}{n}\right)^3 + \frac{2187}{64}.$$

After simple comparison, one has

$$AZI(G_i) > (n-6)\left(\frac{n-2}{n-3}\right)^3 + 64.$$

for $i = 1, 2, \cdots, 5$.

■

Lemma 5. [2] *For a fixed real number p, let*

$$f(x,y) = \left(\frac{xy}{x+y-2}\right)^3 - \left(\frac{y(x-p)}{x+y-p-2}\right)^3,$$

where $x \geq 2$, $x > p \geq 1$ and $y \geq 2$. The function f is increasing in y in the interval $[2, \infty)$.

A *pendent vertex* of a graph is a vertex of degree 1. A vertex adjacent to a vertex $u \in V(G)$ is called a *neighbor* of u.

Lemma 6. *For $n \geq 6$, let G be an n-vertex connected tricyclic graph of maximum degree at most $n-2$ and minimum degree 1. If G is not isomorphic to any of the graphs $H_1, H_2, \cdots, H_6$ shown in Figure 4, then*

$$AZI(G) \geq (n-6)\left(\frac{n-2}{n-3}\right)^3 + 64,$$

with equality if and only if G is isomorphic to the graph G_n^* depicted in Figure 1.

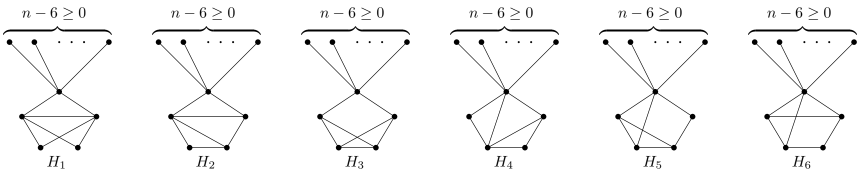

Figure 4. The graphs $H_1, H_2, \cdots, H_6$.

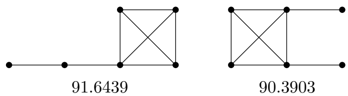

Figure 5. All non-isomorphic connected tricyclic graphs of order 6 satisfying the constraints mentioned in the statement of Lemma 6, together with their approximated AZI.

Proof. This lemma is proved by induction on n. It is noted that there are only two non-isomorphic connected tricyclic graphs of order 6 satisfying the constraints mentioned in the lemma. These two graphs together with their approximated AZI are shown in Figure 5, from which it follows that the lemma holds if $n = 6$, and hence the induction starts. In what follows, it is assumed that $n \geq 7$. Take a vertex $u \in V(G)$ in such a way that the number of pendent vertices adjacent with u is minimum. Suppose that the pendent neighbors of u are $v_1, v_2, \cdots, v_p$ and that the non-pendent neighbors of u are $v_{p+1}, v_{p+2}, \cdots, v_r$. Clearly, $r \geq 2$. Let G' be the graph deduced from G by deleting the vertices $v_1, v_2, \cdots, v_p$. Note that G' has order $n-p$ and size $n-p+2$.

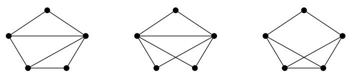

Figure 6. All non-isomorphic connected tricyclic graphs of order 5 and minimum degree at least 2.

If $n-p=5$ then because of the choice of the vertex u and due to the assumption $n \geq 7$ minimum degree of G' is at least 2 (more precisely, it is exactly 2), and so G' must be isomorphic to one of the three graphs shown in Figure 6 and hence G must be isomorphic to one of the six graphs given in Figure 4, which is a contradiction to the definition of G. Thus, $n-p \geq 6$ and hence by inductive hypothesis and Lemma 3, the graph G' satisfies the inequality

$$AZI(G') \geq (n-p-6)\left(\frac{n-p-2}{n-p-3}\right)^3 + 64. \tag{2}$$

where the equality sign in (2) holds if and only if G' is isomorphic to the graph G^*_{n-p} (see Figure 1). Now, if d_{v_i} denotes the degree of the vertex v_i in G for $i = p+1, p+2, \cdots, r$, then by definition of AZI it holds that

$$\begin{aligned} AZI(G) &= \sum_{i=p+1}^{r}\left[\left(\frac{r\, d_{v_i}}{d_{v_i}+r-2}\right)^3 - \left(\frac{(r-p)d_{v_i}}{d_{v_i}+r-p-2}\right)^3\right] \\ &+ p\left(\frac{r}{r-1}\right)^3 + AZI(G'), \end{aligned}$$

which gives the following inequality because of (2) and Lemma 5:

$$AZI(G) \geq p\left(\frac{r}{r-1}\right)^3 + (n-p-6)\left(\frac{n-p-2}{n-p-3}\right)^3 + 64, \tag{3}$$

where the equality sign in (3) holds if and only if $G' \cong G^*_{n-p}$ and $d_{v_i} = 2$ for every $i \in \{p+1, p+2, \cdots, r\}$. Note that the function f defined by $f(x) = \left(\frac{x}{x-1}\right)^3$ with $x \geq 2$, is strictly decreasing in the interval $[2, \infty)$. Thus, the inequality $r \leq n-2$ implies that

$$p\left(\frac{r}{r-1}\right)^3 \geq p\left(\frac{n-2}{n-3}\right)^3, \tag{4}$$

where the equality sign in (4) holds if and only if $r = n-2$. Also, one has

$$\begin{aligned} & p\left(\frac{n-2}{n-3}\right)^3 + (n-p-6)\left(\frac{n-p-2}{n-p-3}\right)^3 + 64 \\ &= AZI(G^*_n) + (n-p-6)\left[\left(\frac{n-p-2}{n-p-3}\right)^3 - \left(\frac{n-2}{n-3}\right)^3\right]. \end{aligned} \tag{5}$$

Since $n-p \geq 6$, it holds that

$$(n-p-6)\left[\left(\frac{n-p-2}{n-p-3}\right)^3 - \left(\frac{n-2}{n-3}\right)^3\right] \geq 0 \tag{6}$$

with equality if and only if $n-p=6$. Therefore, from (3), (4), (5) and (6) it follows that $AZI(G) \geq AZI(G^*_n)$ with equality if and only if G is isomorphic to the graph G^*_n.

■

Lemma 7. *If G is isomorphic to one of the graphs $H_1, H_2, \cdots, H_6$, shown in Figure 4, then*

$$AZI(G) > (n-6)\left(\frac{n-2}{n-3}\right)^3 + 64.$$

Proof. By elementary calculations, one has

$$AZI(H_1) = (n-5)\left(\frac{n-3}{n-4}\right)^3 + 128\left(\frac{n-3}{n-1}\right)^3 + \frac{1376}{27},$$

$$AZI(H_2) = (n-5)\left(\frac{n-3}{n-4}\right)^3 + 27\left(\frac{n-3}{n-2}\right)^3 + 64\left(\frac{n-3}{n-1}\right)^3 + \frac{440309}{8000},$$

$$AZI(H_3) = (n-5)\left(\frac{n-3}{n-4}\right)^3 + 54\left(\frac{n-3}{n-2}\right)^3 + \frac{3645}{64},$$

$$AZI(H_4) = (n-5)\left(\frac{n-2}{n-3}\right)^3 + 27\left(\frac{n-2}{n-1}\right)^3 + 64\left(\frac{n-2}{n}\right)^3 + \frac{5728}{125},$$

$$AZI(H_5) = (n-5)\left(\frac{n-2}{n-3}\right)^3 + 54\left(\frac{n-2}{n-1}\right)^3 + \frac{3211}{64},$$

and

$$AZI(H_6) = (n-5)\left(\frac{n-2}{n-3}\right)^3 + 81\left(\frac{n-2}{n-1}\right)^3 + \frac{1241}{32}.$$

After simple comparison, one has

$$AZI(H_i) > (n-6)\left(\frac{n-2}{n-3}\right)^3 + 64.$$

for $i = 1, 2, \cdots, 6$.

■

Proof of Theorem 1: The result follows directly from Lemmas 3, 4, 6 and 7.

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