Applied Mathematics and Computation 335 (2018) 75–81

Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

Augmented Zagreb index of trees and unicyclic graphs with perfect matchings

Xiaoling Sun[a,b,*], Yubin Gao[a], Jianwei Du[a], Lan Xu[a]

[a] School of Science, North University of China, Taiyuan, Shanxi 030051, PR China
[b] School of Instrument and Electronics, North University of China, Taiyuan, Shanxi 030051, PR China

ARTICLE INFO

MSC:
05C12
92E10

Keywords:
Augmented Zagreb index
Tree
Unicyclic graph
Perfect matching

ABSTRACT

The augmented Zagreb index of a graph G, which is proven to be a valuable predictive index in the study of the heat of formation of octanes and heptanes, is defined as $AZI(G)=\sum_{uv\in E(G)}(\frac{d(u)d(v)}{d(u)+d(v)-2})^3$, 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. In this paper, the lower bounds on augmented Zagreb index of trees and unicyclic graphs with perfect matchings are presented, and the corresponding extremal trees and uinicyclic graphs with perfect matchings are characterized.

1. Introduction

Molecular descriptors have found wide applications in QSPR/QSAR studies. Among them, topological indices have a prominent place [4]. Topological indices are numbers associated with chemical structures derived from their hydrogen-depleted graphs as a tool for compact and effective description of structural formulas which are used to study and predict the structure-property correlations of organic compounds.

We consider non-trivial connected simple graphs only. Such a graph will be denoted by $G=(V(G),E(G))$, where $V(G)$ and $E(G)$ are the vertex set and edge set of G, respectively. Let $N(u)$ denote the set of all neighbors of $u\in V(G)$ in G, and let $d_G(u)=|N(u)|$ ($d(u)$ for short) denote the degree of u. A connected graph without any cycle is a tree. A simple connected graph is called unicyclic if it has exactly one cycle. A vertex u is called a pendent vertex if $d(u)=1$. An edge incident on a pendent vertex is a pendent edge. The graph that arises from G by deleting the vertex $u\in V(G)$ (and its incident edges) or the edge $uv\in E(G)$ will be denoted by $G-u$ or $G-uv$, respectively. Similarly, the graph $G+uv$ arises from G by adding an edge $uv\notin E(G)$ between the endpoints $u,v\in V(G)$. As usual, the cycle and the path of order n is denoted as C_n and P_n, respectively.

A matching M of the graph G is a subset of $E(G)$ such that no two edges in M share a common vertex. If M is a matching of a graph G and vertex $v\in V(G)$ is incident with an edge of M, then v is said to be M-saturated, and if every vertex of G is M-saturated, then M is a perfect matching.

Our other notations are standard and taken mainly from [7].

* Corresponding author at: School of Science, North University of China, Taiyuan, Shanxi 030051, PR China.
E-mail address: sunxiaoling@nuc.edu.cn (X. Sun).

https://doi.org/10.1016/j.amc.2018.04.039
0096-3003/

The augmented Zagreb index (*AZI* for short) was firstly introduced by Furtula et al. in [3], which is defined to be

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

It has been shown that this graph invariant is a valuable predictive index in the study of the heat of formation in octanes and heptanes (see [3]), whose prediction power is better than atom-bond connectivity index (please refer to [1,2,8–12] for its research background). The *AZI* is also related to the well known Randić index (we can see [19,20] on the Randić index).

In [3], Furtula et al. obtained some tight upper and lower bounds for the *AZI* of a chemical tree, and determined the trees of order n with minimal *AZI*. Huang et al. [5] gave some attained upper and lower bounds on the *AZI* and characterized the corresponding extremal graphs. Wang et al. [6] obtained some bounds on the *AZI* of connected graphs by using different graph parameters, and characterized the corresponding graphs. Zhan et al. [13] determined the minimal and the second minimal *AZI* of unicyclic graphs, and determined the minimal *AZI* of bicyclic graphs. For other related results see [14–18].

In this paper, we present the lower bounds on *AZI* of trees and unicyclic graphs with perfect matchings, and characterize the corresponding extremal trees and uinicyclic graphs with perfect matchings.

2. Preliminaries

In this section, we give two useful lemmas.

Lemma 2.1. [5] *Let* $A(x,y) = (\frac{xy}{x+y-2})^3$, *then*

(1) $A(1,y) = (\frac{y}{y-1})^3$ *is decreasing for* $y \geq 2$.

(2) $A(2,y) = 8$ *for* $y \geq 1$.

(3) If $x \geq 3$ *is fixed, then* $A(x, y)$ *is increasing for* $y \geq 1$.

Lemma 2.2. *Let* $f(x,a) = A(x,a) - A(x,a-1)$, *where* x *and* a *are positive integers, and* $a \geq 3$. *Then* $f(x,a) \geq f(2,a) = 0 > f(1,a)$ *for* $x \geq 2$, *and* $f(1, a)$ *is increasing for* a.

Proof. Note that

$$f(x,a) = \frac{(x-2)x^3\big(a^2(a+x-3)^2 + a(a-1)(a+x-2)(a+x-3) + (a-1)^2(a+x-2)^2\big)}{(a+x-2)^3(a+x-3)^3},$$

clearly, for $x \geq 2$, $f(x,a) \geq f(2,a) = 0 > f(1,a)$.

It can be seen that for $a \geq 3$,

$$\begin{aligned}\frac{\mathrm{d}f(1,a)}{\mathrm{d}a} &= \frac{\mathrm{d}}{\mathrm{d}a}\left(\left(\frac{a}{a-1}\right)^3 - \left(\frac{a-1}{a-2}\right)^3\right)\\ &= \frac{3\big(a^2-a-1\big)}{(a-1)^2(a-2)^2}\left(\frac{a-1}{(a-2)^2} + \frac{a}{(a-1)^2}\right) > 0,\end{aligned}$$

so $f(1, a)$ is increasing for a. □

3. Augmented Zagreb index of trees with a perfect matching

In this section, we obtain the lower bound for the *AZI* of trees with a perfect matching.

For positive integer $m \geq 3$, let $\mathbb{T}(m)$ be the set of trees on $2m$ vertices with a perfect matching.

Theorem 3.1. *Let* $T \in \mathbb{T}(m)$, *where* $m \geq 3$. *Then*

$$AZI(T) \geq \begin{cases} \frac{219}{16}m - \frac{91}{16} & if\ m\ is\ odd,\\ \frac{219}{16}m - \frac{295}{64} & if\ m\ is\ even\end{cases}$$

with equality holds if and only if $G \cong T^*_m$ *(where* T^*_m *is depicted in Fig. 3.1).*

Proof. Let

$$\varphi(m) = \begin{cases} \frac{219}{16}m - \frac{91}{16} & if\ m\ is\ odd,\\ \frac{219}{16}m - \frac{295}{64} & if\ m\ is\ even.\end{cases}$$

We prove the result by induction on m.

It is easily seen that $\mathbb{T}(3)$ contains exactly T^*_3 and the path P_6. Note that $AZI(P_6) = 40 > AZI(T^*_3) = \frac{283}{8} = \varphi(3)$, and thus the result holds for $m = 3$. If $m = 4$, then $T \cong T^*_4, P_8$ or H_i $(i = 1, 2, 3,$ see Fig. 3.2). By direct calculation, we can get that