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# Trees with Given Diameter Minimizing the Augmented Zagreb Index and Maximizing the ABC Index

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**Abstract:** Let $G$ be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The augmented Zagreb index of a graph $G$ is defined as

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

and the atom-bond connectivity index (ABC index for short) of a graph $G$ is defined as

$$ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}},$$

where $d_u$ and $d_v$ denote the degree of vertices $u$ and $v$ in $G$, respectively. In this paper, trees with given diameter minimizing the augmented Zagreb index and maximizing the ABC index are determined, respectively.

**Key words:** tree, augmented Zagreb index, ABC index, diameter
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## 1 Introduction

Let $G$ be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. Let $N_u$ denote the set of all neighbors of a vertex $u \in V(G)$, and $d_u = |N_u|$ denote the degree of $u$ in $G$. A connected graph $G$ is called a tree if $|E(G)| = |V(G)| - 1$. The length of a shortest path connecting the vertices $u$ and $v$ in $G$ is called the distance between $u$ and $v$, and denoted by $d(u, v)$. The diameter $d$ of $G$ is the maximum distance $d(u, v)$ over all pairs of vertices $u$ and $v$ in $G$.

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Molecular descriptors have found wide applications in QSPR/QSAR studies (see [1]). Among them, topological indices have a prominent place. Augmented Zagreb index, which was introduced by Furtula *et al.*[2], is a valuable predictive index in the study of the heat of formation in octanes and heptanes. Another topological index, Atom-bond connectivity index (for short, ABC index), proposed by Estrada et al.[3], displays an excellent correlation with the heat of formation of alkanes (see [3]) and strain energy of cycloalkanes (see [4]).

The augmented Zagreb index of a graph $G$ is defined as:

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

and the ABC index of a graph $G$ is defined as:

$$ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}.$$

Some interesting problems such as mathematical-chemical properties, bounds and extremal graphs on the augmented Zagreb index and the ABC index for various classes of connected graphs have been investigated in [2], [5] and [6]–[10], respectively. Besides, in the literature, there are many papers concerning the problems related to the diameter (see, e.g., [11]–[13]). In this paper, trees with given diameter minimizing the augmented Zagreb index and maximizing the ABC index are determined, respectively.

## 2 Trees with Given Diameter Minimizing the Augmented Zagreb Index

A vertex $u$ is called a pendent vertex if $d_u = 1$. Let $S_n$ and $P_n$ denote the star and path of order $n$, respectively. Let $S_l^{n_1,\, n_2}$ be the tree of order $n(\geq 3)$ obtained from the path $P_l$ by attaching $n_1$ and $n_2$ pendent vertices to the end-vertices of $P_l$ respectively, where $l$, $n_1$, $n_2$ are positive integers, $n_1 \leq n_2$ and $l + n_1 + n_2 = n$. Especially, $S_1^{n_3, n-n_3-1} \cong S_n$ and $S_{n-2}^{1,1} \cong P_n$, where $1 \leq n_3 \leq \left\lfloor \frac{n-1}{2} \right\rfloor$.

Let $\mathcal{T}_n^{(d)}$ denote the set of trees with $n$ vertices and diameter $d$, where $2 \leq d \leq n-1$. Obviously, $\mathcal{T}_n^{(2)} = \{S_n\}$ and $\mathcal{T}_n^{(n-1)} = \{P_n\}$. By simply calculating, we have

$$AZI(S_n) = \frac{(n-1)^4}{(n-2)^3}, \qquad AZI(P_n) = 8(n-1).$$

### 2.1 The Augmented Zagreb Index of a Tree with Diameter 3

It can be seen that $\mathcal{T}_n^{(3)} = \left\{ S_2^{p-1, n-p-1} \;\middle|\; 2 \leq p \leq \left\lfloor \frac{n}{2} \right\rfloor \right\}$. In the following, we give an order of the augmented Zagreb index of a tree with diameter 3.

**Lemma 2.1** *Let*

$$g(x) = \frac{x^2}{(x-1)^2}, \qquad k(x) = \frac{-2x^2}{(x-1)^3}, \qquad m(x) = \frac{-3}{x(x-1)} + \frac{-2x+1}{x^2(x-1)^2}.$$

*Then $g(x)$ is decreasing for $x \geq 2$, and $k(x)$, $m(x)$ are both increasing for $x \geq 2$.*