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Some lower and upper bounds on the third ABC index

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Abstract

Atom-bond connectivity (ABC) index has been applied up to now to study the stability of alkanes and the strain energy of cycloalkanes. Graovac defined the second ABC index as

$$ABC_2(G) = \sum_{v_i v_j \in E(G)} \sqrt{\frac{1}{n_i} + \frac{1}{n_j} - \frac{2}{n_i n_j}},$$

and Kinkar studied the upper bounds. In this paper, we define a new index which is called the third ABC index and it is defined as

$$ABC_3(G) = \sum_{v_i v_j \in E(G)} \sqrt{\frac{1}{e_i} + \frac{1}{e_j} - \frac{2}{e_i e_j}}, \tag{1}$$

and we present some lower and upper bounds on ABC_3 index of graphs.

Keywords: Molecular graph; Atom-bond connectivity (ABC) index; The third Atom-bond connectivity (ABC_3) index; Topological indices

1. Introduction

Molecular descriptors are playing significant role in chemistry, pharmacology, etc. Among them, topological indices have a prominent place [1]. One of the best known and widely used index is the connectivity index, χ, introduced in 1975 by Milan Randić [2], who has shown that this index reflects molecular branching. Some novel results about branching can be found in [3–7] and in the references cited therein. However, many physico-chemical properties are dependent on factors other than branching. The lower and upper bounds on ABC index of chemical trees in terms of the number of vertices were obtained in [8]. Also, it has been shown that the star $K_{1,n-1}$, has the maximal ABC value of trees.

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Let $G = (V, E)$ be a simple connected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$, where $|V(G)| = n$ and $|E(G)| = m$. Let $x, y \in V(G)$, then the distance $d_G(x, y)$ between x and y is defined as the length of any shortest path in G connecting x and y. For a vertex v_i of $V(G)$, its eccentricity e_i is the largest distance between v_i and any other vertex v_k of G, i.e, $e_i = max_{v_j \in V(G)} d_G(v_i, v_j)$. The diameter $d(G)$ of G is defined as the maximum eccentricity of G. Similarly, the radius $r(G)$ is defined as the minimum eccentricity of G. There are some topological indices which are related to the eccentricity like the eccentric connectivity index

$$\xi(G) = \sum_{v_i \in V(G)} d_i e_i$$

where d_i is the degree of the vertex v_i.

The Zagreb indices have been introduced more than 30 years ago by Gutman and Trinajstić [9]. They are defined as

$$M_1(G) = \sum_{v_i \in V(G)} d_i^2,$$
$$M_2(G) = \sum_{v_i v_j \in E(G)} d_i d_j.$$

(see [10–13] and the references therein).

Also, there are similar indices called Zagreb eccentricity indices which are also related to eccentricity. Zagreb eccentricity indices are defined as

$$E_1(G) = \sum_{v_i \in V(G)} e_i^2,$$
$$E_2(G) = \sum_{v_i v_j \in E(G)} e_i e_j,$$

(see [14–17] and the references therein).

In order to take this into account but at the same time to keep the spirit of the Randić index, Estrada et al. proposed a new index, nowadays known as the atom-bond connectivity (ABC) index, which is defined as [18]

$$\mathrm{ABC}(G) = \sum_{v_i v_j \in E(G)} \sqrt{\frac{1}{d_i} + \frac{1}{d_j} - \frac{2}{d_i d_j}}.$$

The ABC index has proven to be a valuable predictive index in the study of the heat formation of alkanes [18,19], and some mathematical properties are obtained in [20,21].

Very recently, Graovac [22] defined the second ABC index as

$$\mathrm{ABC}_2(G) = \sum_{v_i v_j \in E(G)} \sqrt{\frac{1}{n_i} + \frac{1}{n_j} - \frac{2}{n_i n_j}},$$

which was given by replacing the vertex degree to n_i, where n_i is the number of vertices of G whose distance to the vertex v_i is smaller than the distance to the vertex v_j. Also, Kinkar establised some mathematical properties of the second ABC index [23].

Now we define the third ABC index; $\mathrm{ABC}_3(G)$,

$$\mathrm{ABC}_3(G) = \sum_{v_i v_j \in E(G)} \sqrt{\frac{1}{e_i} + \frac{1}{e_j} - \frac{2}{e_i e_j}} \tag{2}$$

which was given by replacing the vertex degree to eccentricity, e_i.

In this paper, we present lower and upper bounds on ABC_3 index of connected, simple graphs in terms of other indices; the first Zagreb index, the second Zagreb index, eccentric connectivity index, the first Zagreb eccentricity index, and the second Zagreb eccentricity index.