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On Second Atom−Bond Connectivity Index

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ABSTRACT

The atom-bond connectivity index of graph is a topological index proposed by Estrada et al. as $ABC(G)=\sum_{uv\in E(G)}\sqrt{(d_u+d_v-2)/d_ud_v}$, where the summation goes over all edges of G, d_u and d_v are the degrees of the terminal vertices u and v of edge uv. In the present paper, some upper bounds for the second type of atom-bond connectivity index are computed.

Keywords: atom–bond connectivity index, topological index, star–like graph.

1. INTRODUCTION

All graphs considered in this paper are simple graph and connected. The vertex and edge sets of a graph G are denoted by $V(G)$ and $E(G)$, respectively. A topological index of G is a numeric quantity related to it. In other word, let Λ be the class of connected graphs, then a topological index is a function f: $\Lambda \to R^+$, with this property that if G and H are isomorphic, then $f(G) = f(H)$. Topological indices are important tools in prediction of chemical phenomena, that's why several types of topological indices have been defined. One of them is the atom–bond connectivity index (or ABC index for short). This topological index was proposed by Estrada *et al*. [1] as follows:

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

where the summation goes over all edges $e = uv$ of G and d_u and d_v are degrees of vertices u and v, respectively. For more details about this topological index see references [1–4]. Some upper bounds of ABC index with different parameters have been given in [5]. The properties of ABC index of trees have also been studied in [5–7]. Recently, Graovać and

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Ghorbani, defined a new version of the atom-bond connectivity index namely the second atom–bond connectivity index [8]:

$$ABC_2(G) = \sum_{uv \in E(G)} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}},$$

where n_u is the number of vertices closer to vertex u than vertex v and n_v defines similarly. Some upper and lower bounds of ABC_2 index have been studied in [8]. Throughout this paper, our notations are standard and mainly taken from [9]. In this paper, in the next section, we give the necessary definitions and some preliminary results and in Section 3 we introduce some upper and lower bounds of ABC_2 index with given number of pendent vertices.

2. DEFINITIONS AND PRELIMINARIES

Let K_n, S_n and P_n be the complete graph, star and path on n vertices, respectively. Let also $K_{n,m}$ be the complete bipartite graph on $n + m$ vertices. A tree is said to be star–like if exactly one of its vertices has degree greater than two. By $S(2r,s)$, $r, s \geq 1$, we denote a star–like tree with diameter less than or equal to 4, which has a vertex v_1 of degree $r + s$ and

$$S(2r,s) \setminus \{v_1\} = \underbrace{p_2 \cup \ldots \cup p_2}_{r} \cup \underbrace{p_1 \cup \ldots \cup p_1}_{s}.$$

One can prove that, this tree has $2r + s + 1 = n$ vertices. We say that the star–like tree $S(2r,s)$ has $r + s$ branches, where the lengths of them are $\underbrace{2,\ldots,2}_{r},\underbrace{1,\ldots,1}_{s}$ respectively. For n, $m \geq 2$, denoted by $S_{m,n}$ means a tree with $n + m$ vertices formed by adding a new edge connecting the centers of the stars S_n and S_m. Finally, the complement $\bar{G}$ of a simple graph G is a simple graph with vertex set V and two vertices are adjacent in $\bar{G}$ if and only if they are not adjacent in G.

3. BOUNDS OF ABC$_2$ INDEX

In this section some basic mathematical features of second atom–bond connectivity index are given. A pendent vertex is a vertex of degree one and an edge of a graph is said to be pendant if one of its vertices is a pendent vertex.

Theorem 1. Let G be a connected graph of order n with m edges and p pendent vertices, then

$$ABC_2(G) < p\sqrt{\frac{n-2}{n-1}} + (m-p).$$

Proof. Assume $n \geq 3$. For a pendant edge uv of graph G we have $n_u = 1$, and $n_v = n - 1$. On the other hand, for a non-pendent edge uv $\frac{n_u + n_v - 2}{n_u n_v} < 1$ and so,

$$ABC_2(G) = \sum_{uv \in E} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}} = \sum_{uv \in E, d_u = 1} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}} + \sum_{uv \in E, d_u, d_v \neq 1} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}}$$

$$< p\sqrt{\frac{n-2}{n-1}} + m - p.$$

An easy calculation shows that the Diophantine equation $x + y - 2 = xy$ does not have positive solution and so this bound is not sharp.

□

Theorem 2. Let T a tree of order $n > 2$ with p pendent vertices. Then

$$ABC_2(T) \leq p\sqrt{\frac{n-2}{n-1}} + \frac{\sqrt{2}}{2}(n - p - 1) \tag{1}$$

with equality if and only if $T \cong K_{1,n-1}$ or $T \cong S(2r, s)$, $n = 2r + s + 1$.

Proof. Let T be an arbitrary tree with $n \geq 3$ vertices, for any edge $e = uv$, $n_u + n_v = n$. This implies that

$$ABC_2(T) = \sqrt{n-2} \sum_{uv \in E(T)} \frac{1}{\sqrt{n_u n_v}}.$$

Now we assume that the tree T have p pendent vertices. One can easily prove that for pendant edge $e = uv$, $n_u = 1$, $n_v = n - 1$ and for other edges $2 \leq n_u, n_v \leq n-2$. Hence

$$ABC_2(T) = \sqrt{n-2}\left(\sum_{uv \in E(T), d_u = 1} \frac{1}{\sqrt{n_u n_v}} + \sum_{uv \in E(T), d_u, d_v \neq 1} \frac{1}{\sqrt{n_u n_v}}\right)$$

$$\leq \sqrt{n-2}\left(\frac{p}{\sqrt{n-1}} + \frac{n-p-1}{\sqrt{2(n-2)}}\right) = p\sqrt{\frac{n-2}{n-1}} + \frac{\sqrt{2}}{2}(n-p-1). \tag{2}$$

Suppose now equality holds in equation (1), hence we should consider two following cases:

Case (*a*) $p = n - 1$, in this case for all edges $e = uv$, $n_u = n - 1$, $n_v = 1$ and so $T \cong K_{1,n-1}$.

Case (*b*) $p < n - 1$, in this case the diameter of T is strictly greater than 2. Let a be a pendent vertex. One can easily prove that there is a vertex in $N_G(a)$ such as w adjacent to some non-pendent vertices. Since for all edges $e = wx$ incidence with w, $n_x = n - 2$ and

$n_w = 2$, we conclude that $T \cong S(2r, s)$. Conversely, one can prove that in (1) for two graphs $K_{1,n-1}$ and $S(2r, s)$ ($n=2r+s$) equality holds.

Theorem 3. Let G be a graph on $n > 2$ vertices, m edges and p pendent vertices. Then

$$ABC_2(G) \ge p\sqrt{\frac{n-2}{n-1}}$$

with equality if and only if $G \cong K_{1,n-1}$ or $G \cong K_n$.

Proof. For each pendant edge uv, $n_u = 1$, $n_v = n - 1$ and for the others n_u, $n_v \ge 1$. This implies that

$$ABC_2(G) = \sum_{uv\in E}\sqrt{\frac{n_u+n_v-2}{n_u n_v}} = \sum_{uv\in E, d_u=1}\sqrt{\frac{n_u+n_v-2}{n_u n_v}} + \sum_{uv\in E, d_u, d_v\neq 1}\sqrt{\frac{n_u+n_v-2}{n_u n_v}}$$

$$= p\sqrt{\frac{n-2}{n-1}} + \sum_{uv\in E, d_u, d_v\neq 1}\sqrt{\frac{n_u+n_v-2}{n_u n_v}} \ge p\sqrt{\frac{n-2}{n-1}}.$$

For equality we should consider two cases:

Case(*a*) $p = 0$, in this case for all edges $e = uv$, $n_u = n_v = 1$ and this implies $G \cong K_n$.

Case(*b*) $p = m$, in this case all edges are pendant and so $G \cong K_{1,n-1}$.

Theorem 4. Let T be a tree of order $n > 2$ with p pendent vertices. Then

$$ABC_2(T) \ge p\sqrt{\frac{n-2}{n-1}} + \frac{2\sqrt{n-2}}{n}(n-p-1) \tag{3}$$

with equality if and only if $T \cong K_{1,n-1}$ or $T \cong S_{n/2,n/2}$.

Proof. It is clear that in a tree for every edge uv, $n_u + n_v = n$ and hence

$$ABC_2(T) = \sqrt{n-2}\sum_{uv\in E(T)}\frac{1}{\sqrt{n_u n_v}}.$$

Now we assume that T have p pendent vertices, then there exist p edges such as $e = uv$ where $n_u = 1$ and $n_v = n - 1$. Also, for each non-pendant edge uv, $n_u n_v \le n^2/4$ and so

$$ABC_2(T) = \sqrt{n-2}\left(\sum_{uv \in E(T), d_u = 1} \frac{1}{\sqrt{n_u n_v}} + \sum_{uv \in E(T), d_u, d_v \neq 1} \frac{1}{\sqrt{n_u n_v}}\right)$$

$$= \sqrt{n-2}\left(\frac{p}{\sqrt{n-1}} + \sum_{uv \in E(T), d_u, d_v \neq 1} \frac{1}{\sqrt{n_u n_v}}\right)$$

$$\geq \sqrt{n-2}\left(\frac{p}{\sqrt{n-1}} + \frac{2}{n}(n-p-1)\right) = p\sqrt{\frac{n-2}{n-1}} + \frac{2\sqrt{n-2}}{n}(n-p-1).$$

Let in above formula equality holds, we can consider two following cases:

Case(*a*) $p = n-1$, in this case all edges are pendant. Therefore $T \cong K_{1,n-1}$ and so $ABC_2(T) = \sqrt{(n-1)(n-2)}$.

Case(*b*) $p < n-1$, in this case equality holds if and only if for all non–pendant edges, $n_u = n_v = n/2$ and this completes the proof.

Theorem 5. Let G and $\overline{G}$ are connected graphs on n vertices with p and $\overline{p}$ pendent vertices, respectively. Then

$$ABC_2(G) + ABC_2(\overline{G}) < (p+\overline{p})\left(\sqrt{\frac{n-2}{n-1}} - 1\right) + \binom{n}{2}.$$

Proof. Since $m + \overline{m} = n(n-1)/2$ by using Theorem 1, we get

$$ABC_2(G) + ABC_2(\overline{G}) < p\sqrt{\frac{n-2}{n-1}} + \overline{p}\sqrt{\frac{n-2}{n-1}} + m - p + \overline{m} - \overline{p}$$

$$= (p+\overline{p})\left(\sqrt{\frac{n-2}{n-1}} - 1\right) + \binom{n}{2}.$$

Corollary 6. We have

$$ABC_2(G) + ABC_2(\overline{G}) \geq (p+\overline{p})\sqrt{\frac{n-2}{n-1}}.$$

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