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

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

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

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

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

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

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

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

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

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, $n_v \geq 1$. This implies that

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

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

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

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

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, $n_u n_v \leq n^2/4$ 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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