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Atom-bond connectivity index of graphs

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ABSTRACT

The recently introduced atom-bond connectivity (*ABC*) index has been applied up until now to study the stability of alkanes and the strain energy of cycloalkanes. Furtula et al. (2009) [3] obtained extremal *ABC* values for chemical trees, and also, it has been shown that the star $K_{1,n-1}$, has the maximal *ABC* value of trees. In this paper, we present the lower and upper bounds on *ABC* index of graphs and trees, and characterize graphs for which these bounds are best possible.

1. Introduction

Molecular descriptors play a significant role in chemistry, pharmacology, etc. Among them, topological indices have a prominent place [7]. One of the best known and widely used is the connectivity index, χ, introduced in 1975 by Milan Randić [6], who has shown this index to reflect molecular branching. Some novel results about branching can be found in [4, 8–11] and in the references cited therein. However, many physico-chemical properties are dependent on factors rather different than branching. The lower and upper bounds on ABC index of chemical trees in terms of the number of vertices were obtained in [3]. Also, it has been shown that the star $K_{1,n-1}$, has the maximal ABC value of trees.

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 d_i be the degree of vertex v_i for $i = 1, 2, \ldots, n$. The maximum vertex degree is denoted by Δ, the minimum by δ and the minimum non-pendant vertex degree δ_1. A vertex of a graph is said to be pendant if its neighborhood contains exactly one vertex. An edge of a graph is said to be pendant if one of its vertices is a pendant vertex. The modified second Zagreb index $M_2^*(G)$ is equal to the sum of the products of the reciprocal of the degrees of pairs of adjacent vertices of the underlying molecular graph G, that is, $M_2^*(G) = \sum_{v_iv_j\in E(G)} \frac{1}{d_i\, d_j}$.

In order to take this into account but at the same time to keep the spirit of the Randić index, Ernesto Estrada et al. proposed a new index, nowadays known as the atom-bond connectivity (ABC) index [2]. This index is defined as follows:

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

The ABC index has proven to be a valuable predictive index in the study of the heat of formation in alkanes [1,2].

Let $G = (V, E)$. If $V(G)$ is the disjoint union of two non-empty sets $V_1(G)$ and $V_2(G)$ such that every vertex in $V_1(G)$ has degree r and every vertex in $V_2(G)$ has degree $s(r \geq s)$, then G is an (r, s)-semiregular graph. When $r = s$, it is called a regular graph. If an (r, s)-semiregular graph is a tree, then it is called an $(r, 1)$-semiregular tree.

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The paper is organized is as follows. In Section 2, we present lower and upper bounds on ABC index of connected graph and trees, and characterize graphs for which these bounds are best possible. The bounds of a descriptor are important information of a molecule (graph) in the sense that they establish the approximate range of the descriptor in terms of molecular structural parameters.

2. Lower and upper bounds on ABC index

We refer the reader to the book [5, p. 71–72, 253–255] for a classical result, the Pólya–Szegö inequality. From this result, we can find the following result and it will be used to find the lower bound on ABC index.

Lemma 2.1 ([5]). *Let $(a_1, a_2, \ldots, a_n)$ be positive n-tuples such that there exist positive numbers A, a satisfying:*

$$0 < a \leq a_i \leq A.$$

Then

$$\frac{n\sum_{i=1}^{n} a_i^2}{\left(\sum_{i=1}^{n} a_i\right)^2} \leq \frac{1}{4}\left(\sqrt{\frac{A}{a}} + \sqrt{\frac{a}{A}}\right)^2. \tag{2}$$

The inequality becomes an equality if and only if $a = A$ or

$$q = \frac{A/a}{A/a+1}n$$

is an integer and q of the numbers a_i coincide with a and the remaining $n - q$ of the a_i's coincide with $A\,(\neq a)$.

Let Γ be the class of graphs $H = (V, E)$ such that H is connected graph of minimum vertex degree $\delta = 2$ with q edges $v_iv_j \in E(H)$ such that $d_i = d_j = \Delta\,(\geq 3)$ and the remaining $m - q$ edges $v_iv_j \in E(H)$ such that $d_i = 2$ or $d_j = 2$ or $d_i = d_j = 2$, where Δ is the maximum vertex degree and q is given by

$$q = \frac{m\Delta}{\Delta + 2\sqrt{\Delta - 1}}.$$

We have

$$\mathrm{ABC}(H) = \frac{2m\sqrt{2(\Delta-1)}}{\Delta + 2\sqrt{\Delta-1}}.$$

Now we give a lower bound on ABC(G) of a graph G:

Theorem 2.2. *Let G be a simple connected graph of order n with m edges, p pendant vertices, maximum vertex degree Δ and minimum non-pendant vertex degree δ_1. Then*

$$\mathrm{ABC}(G) \geq p\sqrt{1 - \frac{1}{\delta_1}} + \frac{\sqrt{4(m-p)\left(n - 2M_2^*(G) - p\left(1 - \frac{1}{\Delta}\right)\right)\sqrt{(\Delta-1)(\delta_1-1)}}}{\sqrt{\Delta\delta_1}\left(\frac{1}{\Delta}\sqrt{\Delta-1} + \frac{1}{\delta_1}\sqrt{\delta_1-1}\right)}, \tag{3}$$

where $M_2^*(G)$ is the modified second Zagreb index of G. Moreover, the equality holds if and only if G is isomorphic to a $(\Delta, 1)$-semiregular graph or G is isomorphic to a regular graph or $G \in \Gamma$.

Proof. For $2 \leq \delta_1 \leq d_i, d_j \leq \Delta$, we have

$$\begin{aligned}\frac{1}{d_i} + \frac{1}{d_j} - \frac{2}{d_id_j} &\geq \frac{1}{d_i} + \frac{1}{\Delta}\left(1 - \frac{2}{d_i}\right) \quad \text{as } d_j \leq \Delta \text{ and } 1 - \frac{2}{d_i} \geq 0\\ &= \frac{1}{\Delta} + \frac{1}{d_i}\left(1 - \frac{2}{\Delta}\right)\\ &\geq \frac{2}{\Delta^2}(\Delta - 1), \quad \text{as } d_i \leq \Delta \text{ and } 1 - \frac{2}{\Delta} \geq 0.\end{aligned} \tag{4}$$

For $2 \leq \delta_1 \leq d_i, d_j \leq \Delta$,

$$\frac{1}{d_i} + \frac{1}{d_j} - \frac{2}{d_id_j} \geq \frac{2}{\Delta^2}(\Delta - 1) \tag{5}$$

with equality holding if and only if $d_i = d_j = \Delta$.

Similarly, we can easily show that

$$\frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_id_j}\le\frac{2}{\delta_1^2}(\delta_1-1),\quad \text{for } 2\le\delta_1\le d_i,\ d_j\le\Delta \tag{6}$$

with equality holding if and only if $d_i=d_j=\delta_1$ or $d_i=\delta_1=2$ or $d_j=\delta_1=2$.

Since p is the number of pendant vertices in G, we have $m-p$ number of non-pendant edges in G. By (2), we have

$$\left(\sum_{v_iv_j\in E(G):d_i,d_j\ne 1}\sqrt{\frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_id_j}}\right)^2\ge\frac{4(m-p)\sqrt{(\Delta-1)(\delta_1-1)}}{\Delta\delta_1\left(\frac{1}{\Delta}\sqrt{\Delta-1}+\frac{1}{\delta_1}\sqrt{\delta_1-1}\right)^2}\times\sum_{v_iv_j\in E(G):d_i,d_j\ne 1}\left(\frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_id_j}\right),\quad \text{by (5) and (6)}, \tag{7}$$

that is,

$$\left(\sum_{v_iv_j\in E(G):d_i,d_j\ne 1}\sqrt{\frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_id_j}}\right)^2\ge\frac{4(m-p)\sqrt{(\Delta-1)(\delta_1-1)}}{\Delta\delta_1\left(\frac{1}{\Delta}\sqrt{\Delta-1}+\frac{1}{\delta_1}\sqrt{\delta_1-1}\right)^2}\times\left(n-2M_2^*(G)-\sum_{v_iv_j\in E(G),d_i=1}\left(1-\frac{1}{d_j}\right)\right), \tag{8}$$

that is,

$$\sum_{v_iv_j\in E(G):d_i,d_j\ne 1}\sqrt{\frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_id_j}}\ge\frac{\sqrt{4(m-p)\sqrt{(\Delta-1)(\delta_1-1)}}}{\sqrt{\Delta\delta_1}\left(\frac{1}{\Delta}\sqrt{\Delta-1}+\frac{1}{\delta_1}\sqrt{\delta_1-1}\right)}\sqrt{n-2M_2^*(G)-p\left(1-\frac{1}{\Delta}\right)}. \tag{9}$$

From (1), we get

$$\mathrm{ABC}(G)=\sum_{v_iv_j\in E(G):d_i=1}\sqrt{1-\frac{1}{d_j}}+\sum_{v_iv_j\in E(G):d_i,d_j\ne 1}\sqrt{\frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_id_j}}. \tag{10}$$

Since $1-\frac{1}{d_j}\ge 1-\frac{1}{\delta_1}$ for $d_j\ge\delta_1$, from (10) we get the required result (3), by (9).

Now suppose that equality holds in (3). Then all inequalities in the above argument must be equalities. Now we consider two cases (i) $p>0$, (ii) $p=0$.

Case (i): $p>0$. From $1-\frac{1}{d_j}=1-\frac{1}{\delta_1}$, we get $d_j=\delta_1$ for $v_iv_j\in E$, $d_i=1$.

From equality in (9), we get

$$d_j=\Delta\quad \text{for } v_iv_j\in E(G),\ d_i=1.$$

From these results, we get $\Delta=\delta_1$. Hence G is isomorphic to a $(\Delta,1)$-semiregular graph.

Case (ii): $p=0$. In this case $\delta=\delta_1$. According to the Lemma 2.1, from equality in (7), we get

$$\frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_id_j}=\frac{2}{\Delta^2}(\Delta-1)=\frac{2}{\delta_1^2}(\delta_1-1)\quad \text{for any edge } v_iv_j\in E(G), \tag{11}$$

or

$$\frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_id_j}=\frac{2}{\Delta^2}(\Delta-1)\quad \text{for } q \text{ edges } v_iv_j\in E(G) \tag{12}$$

$$\text{and } \frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_id_j}=\frac{2}{\delta_1^2}(\delta_1-1)\quad \text{for remaining } m-q \text{ edges } v_iv_j\in E(G), \tag{13}$$

where $q=\frac{m\Delta\sqrt{\delta_1-1}}{\Delta\sqrt{\delta_1-1}+\delta_1\sqrt{\Delta-1}}$, and $\frac{2}{\Delta^2}(\Delta-1)\ne\frac{2}{\delta_1^2}(\delta_1-1)$, i.e., $\Delta\ne\delta_1$.

From (11), we get $\Delta=\delta_1$, that is, G is isomorphic to a regular graph.

Otherwise, $\Delta\ne\delta_1$ and we have the relations (12) and (13). First we assume that $\delta_1\ge 3$. From equality in (5) and (6), we get $d_i=d_j=\Delta$ for q edges $v_iv_j\in E(G)$ and $d_i=d_j=\delta_1$ for remaining $m-q$ edges $v_iv_j\in E(G)$. Since G is connected, we have $\Delta = \delta_1$, a contradiction. Thus we may assume that $\delta_1 = 2$. So, $\Delta \geq 3$. From equality in (5) and (6), we get $d_i = d_j = \Delta$ for q edges $v_iv_j \in E(G)$ and for remaining $m - q$ edges $v_iv_j \in E(G)$, $d_i = 2$ or $d_j = 2$ or both $d_i = d_j = 2$, where q is given by

$$q = \frac{m\Delta}{\Delta + 2\sqrt{\Delta - 1}}.$$

Thus $G \in \Gamma$, as G is connected.

Conversely, let G be isomorphic to a $(\Delta, 1)$-semiregular graph. We have

$$\begin{aligned}\mathrm{ABC}(G) &= p\sqrt{1 - \frac{1}{\Delta}} + \frac{\sqrt{4(m-p)\sqrt{(\Delta-1)(\Delta-1)}}}{\Delta\left(\frac{1}{\Delta}\sqrt{\Delta-1} + \frac{1}{\Delta}\sqrt{\Delta-1}\right)}\sqrt{n - 2M_2^*(G) - p\left(1 - \frac{1}{\Delta}\right)}\\ &= p\sqrt{1 - \frac{1}{\Delta}} + (m-p)\sqrt{\frac{2}{\Delta} - \frac{2}{\Delta^2}}.\end{aligned}$$

Let $G \in \Gamma$. Now,

$$\begin{aligned}n - 2M_2^*(G) &= \sum_{v_iv_j \in E(G)} \left(\frac{1}{d_i} + \frac{1}{d_j} - \frac{2}{d_id_j}\right)\\ &= \frac{m\Delta}{\Delta + 2\sqrt{\Delta-1}} \times \frac{2}{\Delta^2}(\Delta - 1) + \frac{2m\sqrt{\Delta-1}}{\Delta + 2\sqrt{\Delta-1}} \times \frac{1}{2}\\ &= \frac{m\sqrt{\Delta-1}}{\Delta}.\end{aligned}$$

Thus

$$\mathrm{ABC}(G) = \frac{2m\sqrt{2(\Delta-1)}}{\Delta + 2\sqrt{\Delta-1}}.$$

Let G be isomorphic to a r-regular graph. Then $\Delta = \delta_1 = r$ and $p = 0$. We have

$$\mathrm{ABC}(G) = \frac{m}{r}\sqrt{2(r-1)}.$$

Hence the theorem. □

Corollary 2.3. *Let T be a tree of order n with p pendant vertices, maximum vertex degree Δ and minimum non-pendant vertex degree δ_1. Then*

$$\mathrm{ABC}(T) \geq p\sqrt{1 - \frac{1}{\delta_1}} + \frac{\sqrt{4(n-1-p)\left(n - 2M_2^*(T) - p\left(1 - \frac{1}{\Delta}\right)\right)\sqrt{(\Delta-1)(\delta_1-1)}}}{\sqrt{\Delta\delta_1}\left(\frac{1}{\Delta}\sqrt{\Delta-1} + \frac{1}{\delta_1}\sqrt{\delta_1-1}\right)}, \tag{14}$$

where $M_2^*(T)$ is the modified second Zagreb index of tree T. Moreover, the equality holds if and only if T is isomorphic to a $(\Delta, 1)$-semiregular tree.

Proof. The proof follows directly from Theorem 2.2. □

Corollary 2.4. *Let T be a tree of order n with p pendant vertices, maximum vertex degree Δ and minimum non-pendant vertex degree δ_1. Then*

$$\mathrm{ABC}(T) \geq \frac{p}{\sqrt{2}} + \frac{\sqrt{4(n-1-p)\left(n - 2M_2^*(T) - p\left(1 - \frac{1}{\Delta}\right)\right)\sqrt{(\Delta-1)(\delta_1-1)}}}{\sqrt{\Delta\delta_1}\left(\frac{1}{\Delta}\sqrt{\Delta-1} + \frac{1}{\delta_1}\sqrt{\delta_1-1}\right)} \tag{15}$$

with equality holding if and only if $T \cong P_n$.

Proof. Since $\delta_1 \geq 2$, from (14), we get the required result (15). Moreover, the equality holds in (15) if and only if T is isomorphic to a $(\Delta, 1)$-semiregular tree and $\delta_1 = 2$, that is, if and only if $T \cong P_n$. □

Now we give another lower bound on ABC(G).

Theorem 2.5. *Let G be a simple connected graph of order n with m edges, maximum vertex degree Δ. Then*

$$\mathrm{ABC}(G) \geq \sqrt{\frac{4m\sqrt{2\Delta}}{\left(\sqrt{\Delta} + \sqrt{2}\right)^2}\left(n - 2M_2^*(G)\right)}, \tag{16}$$

where $M_2^*(G)$ is the modified second Zagreb index of G. Moreover, the equality holds in (16) if and only if $G \cong P_n$ or G is isomorphic to a $(\Delta, 1)$-semiregular graph with number of pendant edges $\frac{\sqrt{2}m}{\sqrt{\Delta}+\sqrt{2}}$.

Proof. Let δ_1 be the minimum non-pendant vertex degree in G. If non-pendant vertex v_j is adjacent to pendant vertex v_i, then

$$\frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_id_j}=1-\frac{1}{d_j}.$$

For $v_iv_j \in E(G)$, $d_i = 1$ and $v_rv_s \in E(G)$, $d_r, d_s \neq 1$, we get

$$\frac{2}{\Delta}-\frac{2}{\Delta^2}\le\frac{1}{d_r}+\frac{1}{d_s}-\frac{2}{d_rd_s}\le\frac{2}{\delta_1}-\frac{2}{\delta_1^2}\le 1-\frac{1}{\delta_1}\le 1-\frac{1}{d_j}\le 1-\frac{1}{\Delta}.$$

Thus

$$\frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_id_j}\le 1-\frac{1}{\Delta} \tag{17}$$

with equality holding if and only if $d_i = 1, d_j = \Delta$ or $d_j = 1, d_i = \Delta$.

Using $a = \frac{2}{\Delta}-\frac{2}{\Delta^2}$, $A = 1-\frac{1}{\Delta}$ and $a_i = \sqrt{\frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_id_j}}$, $i = 1, 2, \ldots, n$ in (2), we get the required result (16). First part of the proof is over.

Now suppose that equality holds in (16). Using same technique as in Theorem 2.2, according to the Lemma 2.1, we get

$$\frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_id_j}=\frac{2}{\Delta^2}(\Delta-1)=1-\frac{1}{\Delta}\quad\text{for any edge } v_iv_j\in E(G), \tag{18}$$

or

$$\frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_id_j}=\frac{2}{\Delta^2}(\Delta-1)\quad\text{for } \frac{\sqrt{\Delta}m}{\sqrt{\Delta}+\sqrt{2}} \text{ edges } v_iv_j\in E(G) \tag{19}$$

and

$$\frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_id_j}=1-\frac{1}{\Delta}\quad\text{for } \frac{\sqrt{2}m}{\sqrt{\Delta}+\sqrt{2}} \text{ edges } v_iv_j\in E(G),\ \Delta\neq 2. \tag{20}$$

From (18), we get $\Delta = 2$, that is, $G \cong P_n$.

Otherwise, $\Delta \neq 2$. From equality in (5) and (19), we get $d_i = d_j = \Delta$ for $\frac{\sqrt{\Delta}m}{\sqrt{\Delta}+\sqrt{2}}$ edges $v_iv_j \in E(G)$. From (17) and (20), we get $d_i = 1, d_j = \Delta$ or $d_j = 1, d_i = \Delta$ for remaining $\frac{\sqrt{2}m}{\sqrt{\Delta}+\sqrt{2}}$ edges $v_iv_j \in E(G)$. Since G is connected, G is isomorphic to a $(\Delta, 1)$-semiregular graph with number of pendant edges $\frac{\sqrt{2}m}{\sqrt{\Delta}+\sqrt{2}}$.

Conversely, one can see easily that the equality holds in (16) for path P_n or $(\Delta, 1)$-semiregular graph with number of pendant edges $\frac{\sqrt{2}m}{\sqrt{\Delta}+\sqrt{2}}$. □

Corollary 2.6. *Let G be a simple connected graph with m edges and maximum vertex degree Δ. Then*

$$\mathrm{ABC}(G)\ge\frac{2^{7/4}m\sqrt{\Delta-1}}{\Delta^{3/4}\left(\sqrt{\Delta}+\sqrt{2}\right)} \tag{21}$$

with equality holding in (21) if and only if $G \cong P_n$.

Proof. Since $\frac{2}{\Delta}-\frac{2}{\Delta^2}$ is the minimum value of $\frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_id_j}$ for all edges $v_iv_j \in E(G)$, we have

$$n-2M^*(G)=\sum_{v_iv_j\in E(G)}\left(\frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_id_j}\right)\ge m\left(\frac{2}{\Delta}-\frac{2}{\Delta^2}\right).$$

Using above result in (16), we get the required result (21). Moreover, the equality holds in (21) if and only if $G \cong P_n$ or G is isomorphic to a $(\Delta, 1)$-semiregular graph with number of pendant edges $\frac{\sqrt{2}m}{\sqrt{\Delta}+\sqrt{2}}$, and

$$\frac{2}{\Delta}-\frac{2}{\Delta^2}=1-\frac{1}{\Delta},$$

that is, if and only if $G \cong P_n$. □

Let Φ_Δ be the class of graphs S_Δ that are connected, whose pendant vertices are adjacent to the maximum degree vertices and all other edges have at least one end-vertex of degree 2. Also let Φ_2 be the class of graphs S_2 that are connected, whose vertices are of degree at least two and all the edges have at least one end-vertex of degree 2. Now we give an upper bound on $\mathrm{ABC}(G)$ of a graph G.

Theorem 2.7. *Let G be a simple connected graph of order n with m edges, p pendant vertices, maximum vertex degree Δ and minimum non-pendant vertex degree δ_1. Then*

$$\mathrm{ABC}(G) \leq p\sqrt{1-\frac{1}{\Delta}} + \frac{m-p}{\delta_1}\sqrt{2(\delta_1-1)} \tag{22}$$

with equality holding if and only if G is isomorphic to a $(\Delta, 1)$-semiregular graph or G is isomorphic to a regular graph or $G \in \Phi_\Delta$ or $G \in \Phi_2$.

Proof. Since $m-p$ number of non-pendant edges in G, by Cauchy–Schwarz inequality, we have

$$\left(\sum_{v_iv_j \in E(G): d_i, d_j \neq 1} \sqrt{\frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_id_j}}\right)^2 \leq (m-p) \sum_{v_iv_j \in E(G): d_i, d_j \neq 1} \left(\frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_id_j}\right) \tag{23}$$

$$\leq \frac{2}{\delta_1^2}(\delta_1-1)(m-p)^2 \quad \text{by (6)}. \tag{24}$$

Since $d_j \leq \Delta$, for any $v_j \in V(G)$, we have

$$1-\frac{1}{d_j} \leq 1-\frac{1}{\Delta}.$$

Using this result in (10), we get the required result (22), by (24).

Now suppose that the equality holds in (22). Then all inequalities in the above argument must be equalities. Then from equality in (23) and (24), for any $v_iv_j \in E(G)$ such that $d_i, d_j \neq 1$, we get

$$\frac{1}{d_i}+\frac{1}{d_j}-\frac{2}{d_id_j} = \frac{2}{\delta_1^2}(\delta_1-1) \quad \text{for } m > p,$$

that is,

$$d_i = d_j = \delta_1 \quad \text{or} \quad d_i = \delta_1 = 2 \quad \text{or} \quad d_j = \delta_1 = 2 \quad \text{for each non-pendant edges } v_iv_j \in E(G).$$

For $p > 0$, we have $d_j = \Delta$, $v_iv_j \in E(G)$, $d_i = 1$.

When $p = 0$, G is isomorphic to a regular graph or $G \in \Phi_2$. When $p > 0$, G is isomorphic to a $(\Delta, 1)$-semiregular graph or $G \in \Phi_\Delta$.

Conversely, let G be isomorphic to a $(\Delta, 1)$-semiregular graph. We have

$$\mathrm{ABC}(G) = p\sqrt{1-\frac{1}{\Delta}} + (m-p)\sqrt{\frac{2}{\Delta^2}(\Delta-1)}.$$

Let G be isomorphic to a r-regular graph. We have

$$\mathrm{ABC}(G) = \frac{m}{r}\sqrt{2(r-1)}.$$

Let $G \in \Phi_\Delta$. We have

$$\mathrm{ABC}(G) = p\sqrt{1-\frac{1}{\Delta}} + \frac{m-p}{\sqrt{2}}.$$

Let $G \in \Phi_2$. We have

$$\mathrm{ABC}(G) = \frac{m}{\sqrt{2}}.$$

Hence the theorem. □

Let Φ_Δ^* be the class of trees S_Δ^*, whose pendant vertices are adjacent to the maximum degree vertices and all other edges have at least one end-vertex of degree 2.

Corollary 2.8. *Let T be a tree of order n with p pendant vertices, maximum vertex degree Δ and minimum non-pendant vertex degree δ_1. Then*

$$\mathrm{ABC}(T) \leq p\sqrt{1-\frac{1}{\Delta}} + \frac{n-p-1}{\delta_1}\sqrt{2(\delta_1-1)} \tag{25}$$

with equality holding if and only if T is isomorphic to a $(\Delta, 1)$-semiregular tree or $T \in \Phi^*_\Delta$.

Proof. The proof follows directly from Theorem 2.7. □

Corollary 2.9 ([3]). *Let T be a tree of order n. Then*

$$\mathrm{ABC}(T) \leq \sqrt{(n-1)(n-2)} \tag{26}$$

with equality holding if and only if $T \cong K_{1,n-1}$.

Proof. Since $\Delta \leq n-1$, from (25), we get

$$\mathrm{ABC}(T) \leq p\sqrt{\frac{n-2}{n-1}} + \frac{n-p-1}{\delta_1}\sqrt{2(\delta_1-1)}. \tag{27}$$

Moreover, the equality holds in (27) if and only if T is isomorphic to a $(\Delta, 1)$-semiregular tree or $T \in \Phi^*_\Delta$ and $\Delta = n-1$, that is, if and only if $T \cong K_{1,n-1}$.

Let us consider a function

$$f(x) = x\sqrt{\frac{n-2}{n-1}} + \frac{n-x-1}{\delta_1}\sqrt{2(\delta_1-1)} \quad \text{for } 0 \leq x \leq n-1.$$

We have

$$f'(x) = \sqrt{\frac{n-2}{n-1}} - \frac{1}{\delta_1}\sqrt{2(\delta_1-1)}.$$

Since $\delta_1 \leq n-1$, we have

$$\frac{\delta_1}{\delta_1-1} \geq \frac{n-1}{n-2}, \qquad \text{i.e., } \frac{2(\delta_1-1)}{\delta_1^2} \leq \frac{n-2}{n-1} \quad \text{as } \delta_1 \geq 2.$$

Using above result we get $f'(x) \geq 0$. Thus $f(x)$ is an increasing function on $[0, n-1]$. Hence we get the required result (26). Moreover, the equality holds in (26) if and only if $T \cong K_{1,n-1}$. □

Remark 2.10. From Corollary 2.9, we conclude that the star, $K_{1,n-1}$, has the maximal ABC value for all trees.

Remark 2.11. The lower and upper bounds given by (3) and (22) are equal when G is isomorphic to a regular graph or G is isomorphic to a $(\Delta, 1)$-semiregular graph.

Remark 2.12. The lower and upper bounds given by (14) and (25) are equal when T is isomorphic to a $(\Delta, 1)$-semiregular tree. Also, the lower and upper bounds given by (14) and (26) are equal when $T \cong K_{1,n-1}$, and the lower and upper bounds given by (15) and (25) are equal when $T \cong P_n$.

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