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Some Lower and Upper Bounds on the Third ABC Co-index

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Abstract: Graonac defined the second ABC index as

$$ABC_2(G) = \sum_{v_iv_j \in E(G)} \sqrt{\frac{1}{n_i} + \frac{1}{n_j} - \frac{2}{n_in_j}}.$$

Dae Won Lee defined the third ABC index as

$$ABC_3(G) = \sum_{v_iv_j \in E(G)} \sqrt{\frac{1}{e_i} + \frac{1}{e_j} - \frac{2}{e_ie_j}}$$

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

$$\overline{ABC_3(G)} = \sum_{v_iv_j \notin E(G)} \sqrt{\frac{1}{n_i} + \frac{1}{n_j} - \frac{2}{n_in_j}}$$

and we found some lower and upper bounds on $\overline{ABC_3(G)}$ index.

Key Words: Molecular graph, the third atom - bond connectivity (ABC_3) index, the third atom - bond connectivity co-index ($\overline{ABC_3}$).

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§1. Introduction

The topological indices plays vital role in chemistry, pharmacology etc [1]. Let $G = (V, E)$ be a simple connected graph with vertex set $V(G) = \{v_1, v_2, \cdots, v_n\}$ and the edge set $E(G)$, with $|V(G)| = n$ and $|E(G)| = m$. Let $u, v \in V(G)$ then the distance between u and v is denoted by $d(u, v)$ and is defined as the length of the shortest path in G connecting u and v.

The eccentricity of a vertex $v_i \in V(G)$ is the largest distance between v_i and any other vertex v_j of G. The diameter $d(G)$ of G is the maximum eccentricity of G and radius $r(G)$ of G is the minimum eccentricity of G.

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The Zagreb indices have been introduced by Gutman and Trinajstic [2]-[5]. They are defined as,

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

The Zagreb co-indices have been introduced by Doslic [6],

$$\overline{M_1(G)} = \sum_{v_i v_j \notin E(G)} (d_i^2 + {d_j}^2), \quad \overline{M_2(G)} = \sum_{v_i v_j \notin E(G)} (d_i d_j).$$

Similarly Zagreb eccentricity indices are defined as

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

Estrada et al. defined atom bond connectivity index [7-10]

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

and Graovac defined second ABC index as

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

which was given by replacing d_i, d_j to n_i, n_j 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 [11-14].

Dae and Wan Lee defined the third ABC index [16]

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

In this paper, we have defined the third ABC co - index; $\overline{ABC_3(G)}$ as

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

found some lower and upper bounds on $\overline{ABC_3(G)}$.

§2. Lower and Upper Bounds on $\overline{ABC_3(G)}$ Index

Calculation shows clearly that

(i) $\overline{ABC_3(K_n)} = 0$;

(ii) $\overline{ABC_3(K_{1,n-1})} = \frac{1}{2}\binom{n}{2}$;

(iii) $\overline{ABC_3(C_{2n})} = 2(n-3)\sqrt{n-2}$;

(iv) $\overline{ABC_3(C_{2n+1})} = n(n-3)\sqrt{\dfrac{4n-12}{(n-1)^2}}$.

Theorem 2.1 *Let G be a simple connected graph. Then $\overline{ABC_3(G)} \geq \frac{1}{\sqrt{\overline{E_2(G)}}}$, where $\overline{E_2(G)}$ is the second zagreb eccentricity coindex.*

Proof Since $G \ncong K_n$, it is easy to see that for every $e = v_iv_j$ in $E(G)$, $e_i + e_j \geq 3$. By the definition of ABC_3 coindex

$$\begin{aligned}\overline{ABC_3(G)} &= \sum_{v_iv_j \notin E(G)} \sqrt{\frac{1}{e_i} + \frac{1}{e_j} - \frac{2}{e_ie_j}} \\ &\geq \sum_{v_iv_j \notin E(G)} \frac{1}{\sqrt{e_ie_j}} \geq \frac{1}{\sqrt{\sum\limits_{v_iv_j \notin E(G)} e_ie_j}} = \frac{1}{\sqrt{\overline{E_2(G)}}}.\end{aligned}$$

□

Theorem 2.2 *Let G be a connected graph with m edges, radius $r = r(G) \geq 2$, diameter $d = d(G)$. Then,*

$$\frac{\sqrt{2m}}{d}\sqrt{d-1} \leq \overline{ABC_3(G)} \leq \frac{\sqrt{2m}}{r}\sqrt{r-1}$$

with equality holds if and only if G is self-centered graph.

Proof For $2 \leq r \leq e_i,\ e_j \leq d$,

$$\begin{aligned}\frac{1}{e_i} + \frac{1}{e_j} - \frac{2}{e_ie_j} &\geq \frac{1}{e_i} + \frac{1}{e_j}(1 - \frac{2}{e_j}) \ \ (\text{as } e_j \leq d,\ 1 - \frac{2}{e_i} \geq 0 = \frac{1}{d} + \frac{1}{e_j}(1 - \frac{2}{d})) \\ &\geq \frac{1}{d} + \frac{1}{d}(1 - \frac{2}{d}) \ (\text{as } e_i \leq d \text{ and } (1 - \frac{2}{d}) \geq 0) \\ &\geq \frac{1}{d} + \frac{1}{d} - \frac{2}{d^2} \\ &\geq \frac{2}{d} - \frac{2}{d^2} \geq \frac{2}{d^2}(d-1)\end{aligned}$$

with equality holds if and only if $e_i = e_j = d$.

Similarly we can easily show that,

$$\frac{1}{e_i} + \frac{1}{e_j} - \frac{2}{e_ie_j} \leq \frac{2}{r^2}(r-1)$$

for $2 \leq r \leq e_i$, $e_j \leq d$ with equality holding if and only if $e_i = e_j = r$. □

The following lemma can be verified easily.

Lemma 2.1 *Let $(a_1, a_2, \cdots, a_n)$ be a positive n-tuple such that there exist positive numbers*

A, a satisfying $0 < a \le a_i \le A$. Then,

$$\frac{n\sum\limits_{i=1}^{n} {a_i}^2}{(\sum\limits_{i=1}^{n} a_i)^2} \le \frac{1}{4}(\sqrt{A/a}+\sqrt{a/A})^2$$

with equality holds if and only if $a = A$ or $q = \dfrac{A/a}{(A/a)+1}n$ is an integer and q of numbers a_i coincide with a and the remaining $n-q$ of the $a_i's$ coincide with $A(\neq a)$.

Theorem 2.3 *Let G be a simple connected graph with m edges, $r = r(G) \ge 2, d = d(G)$. Then,*

$$\overline{ABC_3(G)} = \sqrt{\frac{4m\sqrt{(r-1)(d-1)}}{rd(\frac{1}{r}\sqrt{r-1}+\frac{1}{d}\sqrt{d-1})^2\overline{E2(G)}}}.$$

Proof By Theorem 2.2 we know that

$$\frac{\sqrt{2}}{d}\sqrt{d-1} \le \sqrt{\frac{1}{e_i}+\frac{1}{e_j}-\frac{2}{e_ie_j}} \le \frac{\sqrt{2}}{r}\sqrt{r-1}, \quad v_iv_j \notin E(G). \tag{2.1}$$

Also by Lemma 2.3 we have

$$a \le a_i \le A. \tag{2.2}$$

Let

$$a = \frac{\sqrt{2}}{d}\sqrt{d-1} \text{ and } a_i = \sqrt{\frac{1}{e_i}+\frac{1}{e_j}-\frac{2}{e_ie_j}}, \quad v_iv_j \notin E(G)$$

and

$$A = \frac{\sqrt{2}}{r}\sqrt{r-1}.$$

in equations (2.1) and (2.2). We therefore know that

$$\frac{n\sum\limits_{i=1}^{n} {a_i}^2}{\left(\sum a_i\right)^2} \le \frac{1}{4}\left(\sqrt{\frac{A}{a}}+\sqrt{\frac{a}{A}}\right)^2,$$

i.e.,

$$\frac{\left(\sum a_i\right)^2}{n\sum a_i^2} \ge 4\frac{1}{\left(\sqrt{\frac{A}{a}}+\sqrt{\frac{a}{A}}\right)^2},$$

which implies that

$$\left(\sum a_i\right)^2 \ge \frac{4n\sum a_i^2}{\left(\sqrt{\frac{A}{a}}+\sqrt{\frac{a}{A}}\right)^2} \ge \frac{4n\sum a_i^2}{\left[\frac{\sqrt{A}}{\sqrt{a}}+\frac{\sqrt{a}}{\sqrt{A}}\right]^2} \ge \frac{4n\sum a_i^2}{\left[\frac{A+a}{\sqrt{an}}\right]^2} \ge \frac{4n\sum a_i^2 aA}{[A+a]^2}$$

and

$$\left(\sum_{v_iv_j\in E(G)}\sqrt{\frac{1}{e_i}+\frac{1}{e_j}-\frac{2}{e_ie_j}}\right)^2 \geq \frac{4n\frac{\sqrt{2}}{d}\sqrt{d-1}\frac{\sqrt{2}}{r}\sqrt{r-1}}{\left[\frac{\sqrt{2}}{r}\sqrt{r-1}+\frac{\sqrt{2}}{d}\sqrt{r-1}\right]^2}\sum_{v_iv_j\notin E(G)}\left(\frac{1}{e_i}+\frac{1}{e_j}-\frac{2}{e_ie_j}\right)$$
$$\geq \frac{\frac{8n}{rd}\sqrt{d-1}\sqrt{r-1}}{\frac{2}{r}\left[\frac{\sqrt{r-1}}{r}+\frac{\sqrt{d-1}}{d}\right]^2}\sum_{v_iv_j\notin E(G)}\left(\frac{1}{e_i}+\frac{1}{e_j}-\frac{2}{e_ie_j}\right).$$

Therefore

$$\frac{8n\sqrt{(r-1)(d-1)}}{rd\left[\frac{\sqrt{r-1}}{r}+\frac{\sqrt{d-1}}{d}\right]^2}\sum\left(\frac{1}{e_i}+\frac{1}{e_j}-\frac{2}{e_ie_j}\right) = \frac{\frac{8n}{rd}\sqrt{(r-1)(d-1)}}{\frac{2}{r}\left[\frac{\sqrt{r-1}}{r}+\frac{\sqrt{d-1}}{d}\right]^2}\sum_{v_iv_j}\left(\frac{1}{e_i}+\frac{1}{e_j}-\frac{2}{e_ie_j}\right).$$

We know that

$$\sum_{v_iv_j\notin E(G)}\left(\frac{1}{e_i}+\frac{1}{e_j}-\frac{2}{e_ie_j}\right)\geq \frac{1}{\overline{E_2(G)}}$$

from Theorem 2.1. Thus,

$$\sum_{v_iv_j\notin E(G)}\left(\sqrt{\frac{1}{e_i}+\frac{1}{e_j}-\frac{2}{e_ie_j}}^{\,2}\right)\geq \frac{4m\times\sqrt{(r-1)(d-1)}}{rd\left(\frac{1}{r}\sqrt{r-1}+\frac{1}{d}\sqrt{d-1}\right)}\overline{E_2(G)},$$

$$\sum_{v_iv_j\notin E(G)}\sqrt{\left(\frac{1}{e_i}+\frac{1}{e_j}-\frac{2}{e_ie_j}\right)}\geq\sqrt{\frac{4m\sqrt{(r-1)(d-1)}}{rd\left(\frac{1}{r}\sqrt{r-1}+\frac{1}{d\sqrt{d-1}}\right)\overline{E_2(G)}}}.$$ □

Theorem 2.4 *Let G be a simple connected graph with n vertices and m edges. Then,*

$$\frac{1}{\sqrt{n^2m-n\overline{M_1(G)}+\overline{M_2(G)}}}\leq\overline{ABC_3(G)}\leq\frac{1}{\sqrt{2}}\sqrt{2nm^2-n\overline{M_1(G)}-2m^2}.$$

Proof From Theorem 2.1,

$$\sum_{v_iv_j\notin E(G)}\sqrt{\frac{1}{e_i}+\frac{1}{e_j}-\frac{2}{e_ie_j}}\geq\frac{1}{\sqrt{\sum\limits_{v_iv_j\notin E(G)}e_ie_j}}.$$

Since $e_i\leq(n-d_i)$, we know that

$$\frac{1}{\sqrt{\sum\limits_{v_iv_j\notin E(G)}e_ie_j}}\geq\frac{1}{\sqrt{\sum(n-d_i)(n-d_j)}} = \frac{1}{\sqrt{\sum(n^2-nd_i-nd_j+d_id_j)}}$$
$$= \frac{1}{\sqrt{mn^2-n\overline{M_1(G)}+\overline{M_2(G)}}}.$$

This completes the lower bound.

Now, since $G \ncong K_n$, $e_ie_j \geq 2$ for $v_iv_j \notin E(G)$, we get that

$$\sum_{v_iv_j \notin E(G)} \sqrt{\frac{1}{e_i} + \frac{1}{e_j} - \frac{2}{e_ie_j}} \leq \frac{1}{\sqrt{2}} \sum_{v_iv_j \notin E(G)} \sqrt{e_i + e_j - 2}.$$

By Cachy-Schwarz inequality, we also know that

$$\frac{1}{\sqrt{2}} \sum_{v_iv_j \notin E(G)} \sqrt{e_i + e_j - 2} \leq \frac{1}{\sqrt{2}} \sqrt{\sum_{v_iv_j \notin E(G)} 1 \sum_{v_iv_j \notin E(G)} (e_i + e_j - 2)}.$$

Since $e_i \leq n - d_i$ for $v_i \in V(G)$, we get that

$$\begin{aligned}
&\frac{1}{\sqrt{2}} \sqrt{\sum_{v_iv_j \notin E(G)} 1 \sum_{v_iv_j \notin E(G)} (e_i + e_j - 2)} \\
&\leq \frac{1}{\sqrt{2}} \sqrt{m \sum_{v_iv_j \notin E(G)} (n - d_i + n - d_j - 2)} \\
&\leq \frac{1}{\sqrt{2}} \sqrt{m \left[\sum_{v_iv_j \notin E(G)} 2n - \sum_{v_iv_j \notin E(G)} (d_i + d_j) - 2 \sum_{v_iv_j \notin E(G)} 1 \right]} \\
&= \frac{1}{\sqrt{2}} \sqrt{m \left[2nm - \overline{M_1(G)} - 2m \right]} \\
&= \frac{1}{\sqrt{2}} \sqrt{2m^2n - m\overline{M_1(G)} - 2m^2}.
\end{aligned}$$

□

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