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General Atom-Bond-Connectivity Index of Graphs

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Abstract

The Atom-bond-connectivity index ABC of a graph G is determined by d_i and d_j. In this paper, sharp results for the general ABC index which has chemical applications are found using different methods. These new results for ABC index are investigated in terms of its edges, its vertices and its degrees. In particular, some relations for general ABC index are obtained involving different Topological indices; Randic index, Zagreb index, Harmonic index and Narumi-Katayama index. Indeed, general ABC index is improved by the help of the maximum and minimum degrees.

Keywords: Atom-Bond-Connectivity index, Topological indices, Generalization.

1. Introduction

A topological index is a popular number involved to graph which is used in chemical graph theory, particularly. Topological index also contributes to the design of pharmacologically active compounds and the identification of environmentally hazardous substances. The most important topological indices base on vertex and edge distances. Randic index is used to model the arms of the carbon atom framework of the alkanes. Randic index is described as [2]

$$R(G) = \sum_{v_iv_j \in E(G)} \frac{1}{\sqrt{d_id_j}}$$

where v_iv_j indicates the edge of the graph G and d_i is the degree of the vertex v_i. During many years, different indices are improved. Among them, first and second Zagreb indices are recognized by [4,7]

$$Z_1(G) = \sum_{v_iv_j \in E(G)}(d_i + d_j), Z_2(G) = \sum_{v_iv_j \in E(G)}(d_id_j).$$

Another topological identifier is the Harmonic index that has a prominent place is described in [11]

$$H(G) = \sum_{v_iv_j \in E(G)} \frac{1}{d_i+d_j}$$

A survey of properties of Harmonic index is given in [10,13]. Also the modified Narumi-Katayama index is introduced in [8],

$$NK^*(G) = \prod_{i \in V(G)}(d_i)^{d_i} = \prod_{v_iv_j \in E(G)}(d_id_j).$$

Nowadays, it is found the atom-bond connectivity index ABC which is a good example of linear and branched alkanes with tensile energy of cycloalkanes. ABC index is an important degree based topological index in [9] such that

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

The ABC index plays a significant role in temperature studies in alkanes. [1,3,6] For example, ABC index of ethene (C_2H_4) is $4\sqrt{\frac{2}{3}+\frac{2}{3}}$.

Recently, much attention is being paid to the general ABC index ABC_α is described as

$$ABC_\alpha = ABC_\alpha(G) = \sum_{v_iv_j \in E(G)} \left(\frac{d_i+d_j-2}{d_id_j}\right)^\alpha$$

The narrative order of this study is as follows: In Section 2, some results for general ABC index of graphs with some fixed parameters are obtained. In the sequel, some special bounds are outlined and some inequalities using the vertices, the edges and the degrees are improved. In addition, some novel results for the general ABC index of graphs are pointed out related o Randic index, Zagreb index, Harmonic index and Narumi-Katayama index.

2. Main Results

Let G be a simple, finite, connected graphs with the vertex set $V(G)$ and the edge set $E(G)$. In this section, $\sum_{i,j\in E(G)}$ and $\prod_{i,j\in E(G)}$ is represented by $\sum_{ij}$ and $\prod_{ij}$ respectively.
The article [12] is refered to reader for a classical lemma, the Ozeki's inequality. Also, the following lemma is used to find the bound on general ABC index.

Theorem 2.1. [10] If $\boldsymbol{\alpha \geq 1}$ is an integer and $\boldsymbol{0 \leq x_1 \leq \cdots \leq x_k \leq k-1}$, then

$$(\boldsymbol{k-1})^{\boldsymbol{1-\alpha}} \sum_{\boldsymbol{j=1}}^{\boldsymbol{k}} (\boldsymbol{x^j})^{\boldsymbol{\alpha}} \leq (\sum_{\boldsymbol{j=1}}^{\boldsymbol{k}} (\boldsymbol{x^j})^{\frac{\boldsymbol{1}}{\boldsymbol{\alpha}}})^{\boldsymbol{\alpha}}$$

For details, see [5,14,15].

2.2. On The General ABC Index For $\boldsymbol{\alpha = 1}$ and $\boldsymbol{\alpha = 2}$

In this subsection, G may have several connected components but G does not contain isolated vertices. Here, general ABC index for $\alpha = 1$ is found by adding an edge to G and by deleting an edge from G. Also, special inequalities for general ABC index are established associated with different topological indices.

Theorem 2.2. Let i and j be nonadjacent vertices of graph G and let $G + ij$ be the graph obtained from G by adding edge ij to it. Then,

$i)$ $ABC_1(G+ij) \leq ABC_1(G); d_i \geq 2,$
$ii)$ $ABC_1(G+ij) \geq ABC_1(G); 0 \leq d_i \leq 2.$

Proof: Let $d_i = \mu$ and $d_j = \rho$. For $x, y > 0$,

$$\frac{(\mu+1)+\rho-2}{(\mu+1)y} - \frac{\mu+\rho-2}{\mu\rho} = \frac{-\rho+2}{\mu\rho(\mu+1)}$$

There are two cases in this expression: i) $\rho \geq 2$, ii)$0 < \rho \leq 2$.

Let $i_1, i_2, \ldots, i_k$ be the neighbours of i in G for $k = d_i$ and let $j_1, j_2, \ldots, j_l$ be the neighbours of j in G for $l = d_j$.
Let $\alpha = 1$ in general ABC index.
i) For $\rho \geq 2$; the inequality gives

$$ABC_1(G+ij) - ABC_1(G) = \frac{(d_i+1)+(d_j+1)-2}{(d_i+1)(d_j+1)} + \sum_{m=1}^{k}[\frac{(d_i+1)+d_{i_m}-2}{(d_i+1)(d_{i_m})} - \frac{d_i+d_{i_m}-2}{d_i d_{i_m}}] + \sum_{n=1}^{l}[\frac{(d_j+1)+d_{j_n}-2}{(d_j+1)(d_{j_n})} - \frac{d_j+d_{j_n}-2}{d_j d_{j_n}}] \leq 0$$

ii) Similarly case (i), $ABC_1(G+ij) - ABC_1(G) \geq 0$ for $0 < \rho \leq 2$.

Theorem 2.3. Let i and j be nonadjacent vertices of graph G and let $G - ij$ be the graph obtained from G by deleting edge ij to it. Then,

$i)$ $ABC_1(G) \geq ABC_1(G-ij); d_i \leq 2,$
$ii)$ $ABC_1(G) \leq ABC_1(G-ij); d_i \geq 2.$

Proof: Let $d_i = \mu$ and $d_j = \rho$. For $x > 1, \rho > 0$,

$$\frac{\mu+\rho-2}{\mu\rho} - \frac{(\mu-1)+\rho-2}{(\mu-1)\rho} = \frac{-\rho+2}{\mu\rho(\mu-1)}$$

There are two cases in the above exression:
i) $\rho \geq 2$, ii)$\rho \leq 2$.

Let $i_1, i_2, \ldots, i_k$ be the neighbours of i in G for $k = d_i$ and let $j_1, j_2, \ldots, j_l$ be the neighbours of j in G for $l = d_j$, similar to Theorem 3.1.
Let $\alpha = 1$ in general ABC index.

i) For $\rho \geq 2$; the inequality shows

$$ABC_1(G) - ABC_1(G-ij) = \sum_{m=1}^{k}[\frac{d_i+d_{i_m}-2}{d_i(d_{i_m})} - \frac{(d_i-1)+d_{i_m}-2}{(d_i-1)d_{i_m}}] + \sum_{n=1}^{l}[\frac{d_j+d_{j_n}-2}{d_j(d_{j_n})} - \frac{(d_j-1)+d_{j_n}-2}{(d_j-1)d_{j_n}}] - \frac{(d_i-1)+(d_j-1)-2}{(d_i-1)(d_j-1)} \leq 0$$

ii) Similarly case (i), $ABC_1(G) - ABC_1(G-ij) \geq 0$ for $\rho \leq 2$.

Theorem 2.4. Let G be a nontrivial graph with the minimum degree δ and the maximum degree Δ. Then,

$$ABC_1(G) \geq \frac{\delta m}{\Delta} + (\delta^2 - 2)R^2(G)$$

Proof: It is seen that $(d_i - \delta)(\Delta - d_j) \geq 0$. Thus, $\Delta d_i + \delta d_j \geq d_i d_j$. It is implies that

$$d_i d_j + \Delta\delta \geq \frac{\Delta}{\delta}(d_i + d_j - 2) + \frac{2\Delta}{\delta}$$

Therefore, the inequality gets $1 + \frac{\Delta\delta}{d_i d_j} \leq \frac{\Delta}{\delta}\frac{d_i+d_j-2}{d_i d_j} + \frac{2\Delta}{\delta}\frac{1}{d_i d_j}$. That is; $\frac{\delta m}{\Delta} + (\delta^2-2)\sum_{ij}\frac{1}{d_i d_j} \leq \sum_{ij}\frac{d_i+d_j-2}{d_i d_j}$. By the definition of $ABC_\alpha(G)$ for $\alpha = 1$ and $R(G)$, $ABC_1(G) \geq \frac{\delta m}{\Delta} + (\delta^2-2)R^2(G)$.

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Theorem 2.5. Let G be a nontrivial, regular graph with m edges. Then,

$$ABC_1(G) \geq m\frac{2(NK^*(G))^{\frac{1}{2m}}-2}{NK^*(G)}$$

Proof: By the Aritmetic-Geometric Mean inequality,

$$\frac{1}{m}\sum_{ij}(\frac{d_i+d_j-2}{d_id_j}) \geq \frac{1}{m}\frac{\sum_{ij}(d_i+d_j)-2m}{\sum_{ij}d_id_j}$$
$$\geq \frac{1}{m}\frac{\sum_{ij}2\sqrt{d_id_j-2m}}{\sum_{ij}d_id_j}$$
$$\geq \frac{2(\prod_{ij}\ )^{\frac{1}{m}}-2}{\prod_{ij}\ d_id_j}$$
$$\geq \frac{2(NK^*(G))^{\frac{1}{2m}}-2}{NK^*(G)}$$

Hence,

$$ABC_1(G) \geq m\frac{2(NK^*(G))^{\frac{1}{2m}}-2}{NK^*(G)}$$

Theorem 2.6. Let G be a graph with n vertices and m edges. Then,

$$ABC_2(G) \leq \frac{H^2(G)-4M_2(G)-H(G)+4m}{M_2(G)^2}$$

Proof: Using the definition of $ABC_\alpha(G)$ for $\alpha = 2$; $ABC_2(G)$ is obtained as follows:

$$ABC_\alpha(G) = \sum_{ij}(\frac{d_i+d_j-2}{d_id_j})^\alpha$$
$$\leq \frac{\sum_{ij}(d_i^2+d_j^2)-2\sum_{ij}d_id_j-4\sum_{ij}(d_i+d_j)+\sum 4}{\sum_{ij}(d_id_j)^2}$$
$$\leq \frac{\sum_{ij}(d_i+d_j)^2-4\sum_{ij}d_id_j-\sum_{ij}(d_i+d_j)+4m}{M_2(G)^2}$$
$$= \frac{H^2(G)-4M_2(G)-H(G)+4m}{M_2(G)^2}$$

2.2. On The General ABC Index

In this subsection, ABC index is generalized and some relations for general ABC index are obtained consepting the degrees.

Theorem 2.7. Let G be a nontrivial graph with $x, y \in \mathbb{R}$. Then,

$$ABC_{x+y}(G)ABC_{x-y}(G)-\sigma_{x,y} \leq ABC_x(G) \leq \sqrt{ABC_{x+y}(G)ABC_{x-y}(G)}$$

with

$$\sigma_{x,y} = \begin{cases} 2^{x-2}n^2(\left(\frac{\delta-1}{\delta^2}\right)^x - \left(\frac{\Delta-1}{\Delta^2}\right)^x) & ;\ if\ |x| \geq |y| \\ 2^{x-2}n^2(\left(\frac{\Delta-1}{\Delta^2}\right)^{\frac{x+y}{2}}\left(\frac{\delta-1}{\delta^2}\right)^{\frac{x-y}{2}} - \left(\frac{\delta-1}{\delta^2}\right)^{\frac{x+y}{2}}\left(\frac{\Delta-1}{\Delta^2}\right)^{\frac{x-y}{2}}) & ;\ if\ |x| < |y| \end{cases}$$

Proof: The Cauchy-Schwarz inequality gives that

$$\sum_{ij}(\frac{d_i+d_j-2}{d_id_j})^\alpha = \sum_{ij}(\frac{d_i+d_j-2}{d_id_j})^{\frac{x+y}{2}+\frac{x-y}{2}}$$
$$\leq \sum_{ij}((\frac{d_i+d_j-2}{d_id_j})^{x+y})^{\frac{1}{2}}\sum_{ij}((\frac{d_i+d_j-2}{d_id_j})^{x-y})^{\frac{1}{2}}$$
$$= \sqrt{ABC_{x+y}(G)ABC_{x-y}(G)}$$

In this expression, there are four cases:

1) If $x+y \geq 0$ then, $(\frac{2\Delta-2}{\Delta^2})^{\frac{x+y}{2}} \leq (\frac{d_i+d_j-2}{d_id_j})^{\frac{x+y}{2}} \leq (\frac{2\delta-2}{\delta^2})^{\frac{x+y}{2}}$.

2) If $x+y \leq 0$ then, $(\frac{2\delta-2}{\delta^2})^{\frac{x+y}{2}} \leq (\frac{d_i+d_j-2}{d_id_j})^{\frac{x+y}{2}} \leq (\frac{2\Delta-2}{\Delta^2})^{\frac{x+y}{2}}$.

3) If $x-y \geq 0$ then, $(\frac{2\Delta-2}{\Delta^2})^{\frac{x-y}{2}} \leq (\frac{d_i+d_j-2}{d_id_j})^{\frac{x-y}{2}} \leq (\frac{2\delta-2}{\delta^2})^{\frac{x-y}{2}}$.

4) If $x-y \leq 0$ then, $(\frac{2\delta-2}{\delta^2})^{\frac{x-y}{2}} \leq (\frac{d_i+d_j-2}{d_id_j})^{\frac{x-y}{2}} \leq (\frac{2\Delta-2}{\Delta^2})^{\frac{x-y}{2}}$.

Let $(x+y)(x-y) \geq 0$. By the Ozeki's inequality, it is seen that

$$\sum_{ij}((\frac{d_i+d_j-2}{d_id_j})^{\frac{x+y}{2}})^2\sum_{ij}((\frac{d_i+d_j-2}{d_id_j})^{\frac{x-y}{2}})^2$$
$$-(\sum_{ij}\left(\frac{d_i+d_j-2}{d_id_j}\right)^{\frac{x+y}{2}}\sum_{ij}\left(\frac{d_i+d_j-2}{d_id_j}\right)^{\frac{x-y}{2}})^2$$
$$\leq \frac{n^2}{4}(\left(\frac{2\delta-2}{\delta^2}\right)^{\frac{x+y}{2}}\left(\frac{2\delta-2}{\delta^2}\right)^{\frac{x-y}{2}} - \left(\frac{2\Delta-2}{\Delta^2}\right)^{\frac{x+y}{2}}\left(\frac{2\Delta-2}{\Delta^2}\right)^{\frac{x-y}{2}})$$

and thus,

$$ABC_{x+y}(G)ABC_{x-y}(G)-ABC_x(G) \leq 2^{x-2}n^2(\left(\frac{\delta-1}{\delta^2}\right)^x - \left(\frac{\Delta-1}{\Delta^2}\right)^x).$$

It follows that

$$ABC_{x+y}(G)ABC_{x-y}(G)-\sigma_{x,y} \leq ABC_x(G).$$

Let $(x+y)(x-y)<0$. It is represented that

$$ABC_{x+y}(G)ABC_{x-y}(G)-ABC_x(G) \leq \frac{n^2}{4}\left(\left(\frac{2\Delta-2}{\Delta^2}\right)^{\frac{x+y}{2}}\left(\frac{2\delta-2}{\delta^2}\right)^{\frac{x-y}{2}} - \left(\frac{2\delta-2}{\delta^2}\right)^{\frac{x+y}{2}}\left(\frac{2\Delta-2}{\Delta^2}\right)^{\frac{x-y}{2}}\right)$$

And thus,

$$ABC_{x+y}(G)ABC_{x-y}(G)-2^{x-2}n^2\left(\left(\frac{\Delta-1}{\Delta^2}\right)^{\frac{x+y}{2}}\left(\frac{\delta-1}{\delta^2}\right)^{\frac{x-y}{2}} - \left(\frac{\delta-1}{\delta^2}\right)^{\frac{x+y}{2}}\left(\frac{\Delta-1}{\Delta^2}\right)^{\frac{x-y}{2}}\right) \leq ABC_x(G).$$

Hence,
$ABC_x(G) \geq ABC_{x+y}(G)ABC_{x-y}(G)-\sigma_{x,y}.$

Theorem 2.9. Let G be a nontrivial graph with m edges, maximum degree Δ and $2\Delta \leq m-1$. For any integer $4\alpha \geq 1$,

$$ABC_\alpha(G) \leq \delta^\alpha R_\alpha(G)+\alpha\delta^{\alpha-2}R_{\alpha-1}(G).$$

Proof: It is seen that $(d_i-\delta)(d_j-\delta)\geq 0$. Hence, $(d_id_j+\delta^2)\geq \delta(d_i+d_j-2)$. That is; $(\frac{d_id_j}{\delta^2}+1)^\alpha \geq \delta^{-\alpha}(d_i+d_j-2)^\alpha$.
By the Bernoulli inequality for $x\geq -1$, it gives that

$\delta^{-\alpha}(d_i+d_j-2)^\alpha \leq \left(\frac{d_id_j}{\delta^2}+1\right)^\alpha \leq 1+\alpha\frac{d_id_j}{\delta^2}$. Thus, $\frac{(d_i+d_j-2)^\alpha}{(d_id_j)^\alpha} \leq \frac{\delta^\alpha+\alpha\delta^{\alpha-2}d_id_j}{(d_id_j)^\alpha}$
$(\frac{d_i+d_j-2}{d_id_j})^\alpha \leq \frac{\delta^\alpha}{(d_id_j)^\alpha}+\frac{\alpha\delta^{\alpha-2}}{(d_id_j)^{\alpha-1}}$.
$\sum_{ij}(\frac{d_i+d_j-2}{d_id_j})^\alpha \leq$
$\delta^\alpha\sum_{ij}\frac{1}{(d_id_j)^\alpha}+\alpha\delta^{\alpha-2}\sum_{ij}\frac{1}{(d_id_j)^{\alpha-1}}$.

Therefore,

$$ABC_\alpha(G) \leq \delta^\alpha R_\alpha(G)+\alpha\delta^{\alpha-2}R_{\alpha-1}(G).$$

3. Conclusion

$\boldsymbol{ABC}$ index is an important estimation index in chemical graph theory. In this paper, some effects for the $\boldsymbol{ABC}$ index and the general $\boldsymbol{ABC}$ index are formed by the help of degrees and different topological indices. This paper aims to contribute to the use of the $\boldsymbol{ABC}$ index.

Author's Contributions

Seda Kınacı: Prepared and wrote the draft, proved the theorems.

Ethics

In the creation of this article, ethical violations were taken into account and acted within this framework.

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