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A NOTE ON
ATOM - BOND CONNECTIVITY INDEX OF GRAPHS

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Abstract. Let $G = (V, E)$, $V = \{1, 2, \dots, n\}$, be a simple connected graph with n vertices, m edges and sequence of vertex degrees $\Delta = d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n = \delta > 0$, $d_i = d(i)$. With $i \sim j$ we denote the adjacency of the vertices i and j in G. The atom–bond connectivity index of G is defined as $ABC = \sum_{i\sim j} \sqrt{\frac{d_i+d_j-2}{d_id_j}}$. In this note we obtain some new bounds for the ABC index.

1. Introduction

Let $G = (V, E)$, $V = \{1, 2, \dots, n\}$, $E = \{e_1, e_2, \dots, e_m\}$, be a simple connected graph with n vertices and m edges. The number of the first neighbors of the vertex i is called the degree of this vertex and is denoted by $d_i = d(i)$. The degree of an edge $e \in E$ connecting the vertices i and j is defined as $d(e) = d_i + d_j - 2$. Denote by $\Delta = d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n = \delta > 0$, and $d(e_1) \geqslant d(e_2) \geqslant \cdots \geqslant d(e_m)$ sequences of vertex and edge degrees, respectively. If vertices i and j are adjacent we write $i \sim j$. As usual, $L(G)$ denotes a line graph of a graph G. With Γ_2 we denote a class of simple connected graphs in which every edge is incident with at least one vertex of degree 2.

A topological index, or graph invariant, for a graph is a numerical quantity which is invariant under isomorphism of the graph. Very often in chemistry the aim is the construction of chemical compounds with certain properties, which not only depend on the chemical formula but also strongly on the molecular structure. That is where various topological indices come into consideration. Hundreds of different invariants have been employed to date, with varying success, in QSAR (quantitative structure-activity relationships) and QSPR (quantitative structure-property relationships) studies. There is lot of research which is done in this area in the last few decades.

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Two vertex-degree–based topological indices, the first and the second Zagreb index, M_1 and M_2, are defined as

$$M_1 = M_1(G) = \sum_{i=1}^{n} d_i^2 \quad \text{and} \quad M_2 = M_2(G) = \sum_{i\sim j} d_i d_j .$$

The quantity M_1 was first time considered in 1972 [**6**], whereas M_2 in 1975 [**7**]. These are among the most thoroughly examined vertex-degree-based topological indices. Details of the theory and applications of the two Zagreb indices can be found in surveys [**1**, **3**, **8**, **12**, **14**] and in the references cited therein.

Generalization of the second Zagreb index, reported in [**2**], known as general Randić index, R_α, is defined as

$$R_\alpha = R_\alpha(G) = \sum_{i\sim j} (d_i d_j)^\alpha ,$$

where α is an arbitrary real number. Here we are interested in the special case $\alpha = -1$, that is

$$R_{-1} = R_{-1}(G) = \sum_{i\sim j} \frac{1}{d_i d_j}$$

proposed in [**14**] under the name modified second Zagreb index.

Multiplicative versions of the first and the second Zagreb indices, Π_1 and Π_2, were first considered in [**16**] published in 2011, and were promptly followed by numerous additional studies. These indices are defined as:

$$\Pi_1 = \Pi_1(G) = \prod_{i=1}^{n} d_i^2 \quad \text{and} \quad \Pi_2 = \Pi_2(G) = \prod_{i\sim j} d_i d_j .$$

The atom-bond connectivity index, introduced in [**4**], which is conveniently abbreviated by ABC, is defined as

$$ABC = ABC(G) = \sum_{i\sim j} \sqrt{\frac{d_i + d_j - 2}{d_i d_j}} .$$

It was shown [**4**, **5**, **9**] that the ABC index is excellently correlated with the thermodynamic properties of alkanes, especially with their heats of formation.

In this note we obtain lower and upper bounds for the ABC index in terms of some of the main graph parameters and above mentioned indices. Before this, we need to recall a few results from the literature that are of interest for our work.

2. Preliminaries

Let $a = (a_i)$, $i = 1, 2, \dots, m$, be a positive real number sequence. In [**11**] the following double inequality was proven

$$\sum_{i=1}^{m} a_i + m(m-1) \left(\prod_{i=1}^{m} a_i \right)^{\frac{1}{m}} \leqslant \left(\sum_{i=1}^{m} \sqrt{a_i} \right)^2 \leqslant (m-1) \sum_{i=1}^{m} a_i + m \left(\prod_{i=1}^{m} a_i \right)^{\frac{1}{m}} . \tag{2.1}$$

Equalities hold if and only if $a_1 = a_2 = \cdots = a_m$.

In [**17**] and [**10**], respectively, the following upper bound on $ABC(G)$ were determined

$$ABC(G) \leqslant \sqrt{m(n-2R_{-1}(G))}\,, \tag{2.2}$$

and

$$ABC(G) \leqslant \sqrt{m\left(n-\frac{2m^2}{M_2(G)}\right)}, \tag{2.3}$$

Also, both in [**10**] and [**17**] it was proven that

$$ABC(G) \leqslant \sqrt{m\left(n-\frac{4m}{4m+1-\sqrt{8m+1}}\right)}. \tag{2.4}$$

3. Main results

In the following theorem we determine lower and upper bounds for ABC index in terms of parameters n, m and invariants Π_1 and Π_2.

THEOREM 3.1. *Let G be a simple connected graph with $n \geqslant 2$ vertices and m edges. Then*

$$\begin{aligned} &\left(n-2R_{-1}(G)+m(m-1)\frac{\Pi_1(L(G))^{\frac{1}{2m}}}{\Pi_2(G)^{\frac{1}{m}}}\right)^{\frac{1}{2}} \leqslant ABC(G) \\ &\leqslant \left((m-1)(n-2R_{-1}(G))+m\frac{\Pi_1(L(G))^{\frac{1}{2m}}}{\Pi_2(G)^{\frac{1}{m}}}\right)^{\frac{1}{2}}. \end{aligned} \tag{3.1}$$

Equalities hold if and only if $G \in \Gamma_2$ or G is regular or semiregular bipartite graph.

PROOF. For $a_i = \frac{d_i+d_j-2}{d_id_j}$, where summation is performed over all adjacent vertices i and j in G, the inequality (2.1) becomes

$$\begin{aligned} &\sum_{i\sim j}\frac{d_i+d_j-2}{d_id_j}+m(m-1)\left(\prod_{i\sim j}\frac{d_i+d_j-2}{d_id_j}\right)^{\frac{1}{m}} \leqslant \left(\sum_{i\sim j}\sqrt{\frac{d_i+d_j-2}{d_id_j}}\right)^2 \\ &\leqslant (m-1)\sum_{i\sim j}\frac{d_i+d_j-2}{d_id_j}+m\left(\prod_{i\sim j}\frac{d_i+d_j-2}{d_id_j}\right)^{\frac{1}{m}}. \end{aligned} \tag{3.2}$$

The following identities hold

$$\sum_{i\sim j}\frac{d_i+d_j-2}{d_id_j}=\sum_{i\sim j}\left(\frac{1}{d_i}+\frac{1}{d_i}\right)-2\sum_{i\sim j}\frac{1}{d_id_j}=n-2R_{-1}(G)$$

and

$$\prod_{i\sim j}\frac{d_i+d_j-2}{d_id_j}=\frac{\prod_{i\sim j}(d_i+d_j-2)}{\prod_{i\sim j}d_id_j}=\frac{\prod_{i=1}^{m}d(e_i)}{\Pi_2(G)}=\frac{\Pi_1(L(G))^{\frac{1}{2}}}{\Pi_2(G)}.$$

According to the above and (3.2) we arrive at (3.1).

Equalities in (3.2) hold if and only if for any two adjacent edges $ij, iv \in E(G)$ we have that

$$\frac{d_i + d_j - 2}{d_i d_j} = \frac{d_i + d_v - 2}{d_i d_v},$$

that is

$$(d_i - 2)(d_i - d_j) = 0\,.$$

This means that equalities in (3.1) hold if and only if $G \in \Gamma_2$ or G is regular or semiregular bipartite graph. □

Remark 3.1. Since

$$n - 2R_{-1}(G) = \sum_{i\sim j} \frac{d_i + d_j - 2}{d_i d_j} \geqslant m \frac{\Pi_1(L(G))^{\frac{1}{2m}}}{\Pi_2(G)^{\frac{1}{m}}},$$

it follows

$$(m-1)(n - 2R_{-1}(G)) + m\frac{\Pi_1(L(G))^{\frac{1}{2m}}}{\Pi_2(G)^{\frac{1}{m}}} \leqslant m(n - 2R_{-1}(G))\,.$$

Consequently the right-hand side of (3.1) is stronger than (2.2).

Corollary 3.1. *Let G be a simple connected graph with $n \geqslant 2$ vertices and m edges. Then*

$$ABC(G) \leqslant \left((m-1)\left(n - \frac{2m^2}{M_2(G)}\right) + m\frac{\Pi_1(L(G))^{\frac{1}{2m}}}{\Pi_2(G)^{\frac{1}{m}}}\right)^{\frac{1}{2}}. \tag{3.3}$$

Equality holds if and only if G is regular or semiregular bipartite graph.

Proof. Using the arithmetic-harmonic mean inequality for real numbers (see e.g. [**13**]), we have

$$R_{-1}(G)M_2(G) \geqslant m^2.$$

From the above and (3.1) we obtain (3.3). □

Remark 3.2. The inequality (3.3) is stronger than (2.3).

Corollary 3.2. *Let G be a simple connected graph with $n \geqslant 2$ vertices and m edges. Then*

$$ABC(G) \leqslant \left((m-1)\left(n - \frac{4m}{4m+1-\sqrt{8m+1}}\right) + m\frac{\Pi_1(L(G))^{\frac{1}{2m}}}{\Pi_2(G)^{\frac{1}{m}}}\right)^{\frac{1}{2}}. \tag{3.4}$$

Equality holds if and only if $G \cong K_n$.

Proof. In [**2**] it was proven

$$R_{-1}(G) \geqslant \frac{2m}{4m+1-\sqrt{8m+1}}.$$

From the above and (3.1) we obtain (3.4). □

Remark 3.3. The inequality (3.4) is stronger than (2.4).

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