

## On atom–bond connectivity index

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**Abstract.** The atom–bond connectivity index (*ABC*) is a vertex–degree based graph invariant, put forward in the 1990s, having applications in chemistry. Let  $G = (V, E)$  be a graph,  $d_i$  the degree of its vertex  $i$ , and  $ij$  the edge connecting the vertices  $i$  and  $j$ . Then  $ABC = \sum_{ij \in E} \sqrt{(d_i + d_j - 2)/(d_i d_j)}$ . Upper bounds and Nordhaus–Gaddum type results for *ABC* are established.

### 1. Introduction

Several graph invariants found applications and are currently used in chemistry, pharmacology, environmental sciences, etc. [10, 15, 16]. One of these is the so-called “atom–bond connectivity index” (*ABC*). It is defined as follows [6].

Let  $G = (V(G), E(G))$  be a graph with  $n = |V(G)|$  vertices and  $m = |E(G)|$  edges. The degree (= number of first neighbors) of a vertex  $i \in V(G)$  is denoted by  $d_i$ . The edge connecting the vertices  $i$  and  $j$  is denoted by  $ij$ . Then

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

In [6] it was shown that *ABC* can be used for modeling thermodynamic properties of organic chemical compounds. However, this paper did not receive much attention. In 2008, Estrada published another paper, applying *ABC* as tool for explaining the stability of branched alkanes [5]. Contrary to [6], this work attracted the attention of mathematically oriented scholars, resulting in a remarkable number of researches on the mathematical properties of the *ABC* index [1–4, 7–9, 12, 17–19]. In the present paper we report a few more, hitherto unpublished, results on *ABC*.

We first define the graph theoretic notions that will be used in the subsequent parts of the paper.

The maximal and minimal vertex degree of the graph  $G = (V(G), E(G))$  is denoted by  $\Delta$  and  $\delta$ , respectively. A vertex  $i$  is said to be pendent if  $d_i = 1$ . The minimal degree of a non-pendent vertex is  $\delta_1$ . An edge of a graph is said to be pendent if one of its end-vertices is pendent.

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The set of first neighbors of the vertex  $i$  is denoted by  $N_i$ . Evidently,  $|N_i| = d_i$ .

The Zagreb indices are well-known graph invariants, introduced almost 40 years ago [15, 16], defined as:

$$M_1 = M_1(G) = \sum_{i \in V(G)} d_i^2 \quad \text{and} \quad M_2 = M_2(G) = \sum_{ij \in E(G)} d_i d_j.$$

A recently proposed variant of the second Zagreb index, denoted by  $M_2^*$  and defined as [13]:

$$M_2^* = M_2^*(G) = \sum_{ij \in E(G)} \frac{1}{d_i d_j}$$

is known under the name “modified second Zagreb index”.

If  $V(G)$  is the disjoint union of two nonempty 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  $s$  ( $r \leq s$ ), then  $G$  is  $(r, s)$ -semiregular. If  $r = s$ , then  $G$  is said to be regular. As usual [11], the complete graph, complete bipartite graph, the star, and the path are denoted as  $K_n$ ,  $K_{p,q}$  ( $p + q = n$ ),  $K_{1,n-1}$ , and  $P_n$ , respectively.

## 2. Upper bound on ABC index

Upper bounds for the ABC index were earlier obtained in [2, 3]. In particular, inequality (2) was reported in [3], but without the characterization of the equality cases (which seems to be its most difficult aspect).

Our starting point is the well-known Cauchy–Schwarz inequality:

**Lemma 2.1.** *If  $\bar{a} = (a_1, a_2, \dots, a_n)$  and  $\bar{b} = (b_1, b_2, \dots, b_n)$  are sequences of real numbers, then*

$$\left( \sum_{i=1}^n a_i b_i \right)^2 \leq \sum_{i=1}^n a_i^2 \sum_{i=1}^n b_i^2$$

with equality if and only if the sequences  $\bar{a}$  and  $\bar{b}$  are proportional, i. e., there is a  $\lambda \in \mathbb{R}$  such that  $a_k = \lambda b_k$  for each  $k \in \{1, 2, \dots, n\}$ .

**Theorem 2.2.** *Let  $G$  be a connected graph with  $n$  vertices,  $p$  pendent vertices,  $m$  edges, maximal degree  $\Delta$ , and minimal non-pendent vertex degree  $\delta_1$ . Let  $M_1$  and  $M_2^*$  be the first and modified second Zagreb indices of  $G$ . Then*

$$ABC(G) \leq p \sqrt{1 - \frac{1}{\Delta}} + \sqrt{[M_1 - 2m - p(\delta_1 - 1)] \left( M_2^* - \frac{p}{\Delta} \right)}. \tag{2}$$

Equality in (2) holds if and only if  $G$  is regular or  $(1, \Delta)$ -semiregular or bipartite semiregular.

Recall that for  $r \neq s$ , a graph  $G$  is said to be  $(r, s)$ -semiregular if its vertex degrees assume only the values  $r$  and  $s$ , and if there is at least one vertex of degree  $r$  and at least one of degree  $s$ . If every vertex of degree  $r$  is adjacent to vertices of degree  $s$  and vice versa, then  $G$  is bipartite  $(r, s)$ -semiregular. In Theorem 2.2, under “bipartite semiregular” is meant bipartite  $(r, s)$ -semiregular with arbitrary  $r$  and  $s$ .

*Proof.* Using  $a_{ij} = \sqrt{d_i + d_j - 2}$  and  $b_{ij} = 1 / \sqrt{d_i d_j}$ , for each edge  $ij \in E(G)$ , such that both vertex degrees  $d_i$

and  $d_j$  are greater than unity, in Lemma 2.1, we get

$$\left( \sum_{\substack{ij \in E(G) \\ d_i, d_j \neq 1}} \sqrt{\frac{d_i + d_j - 2}{d_i d_j}} \right)^2 = \left( \sum_{\substack{ij \in E(G) \\ d_i, d_j \neq 1}} \frac{\sqrt{d_i + d_j - 2}}{\sqrt{d_i d_j}} \right)^2$$

$$\leq \sum_{\substack{ij \in E(G) \\ d_i, d_j \neq 1}} (d_i + d_j - 2) \sum_{\substack{ij \in E(G) \\ d_i, d_j \neq 1}} \frac{1}{d_i d_j} \tag{3}$$

$$= \left( \sum_{ij \in E(G)} (d_i + d_j - 2) - \sum_{\substack{ij \in E(G) \\ d_i=1}} (d_j - 1) \right) \left( \sum_{ij \in E(G)} \frac{1}{d_i d_j} - \sum_{d_i=1} \frac{1}{d_j} \right)$$

$$\leq [M_1 - 2m - p(\delta_1 - 1)] \left( M_2^* - \frac{p}{\Delta} \right) \tag{4}$$

since  $\sum_{ij \in E(G)} (d_i + d_j) = M_1$  and  $\delta_1 \leq d_i \leq \Delta$ . Therefrom inequality (2) follows directly from the definition (1).

The examination of the equality case in (2) is somewhat lengthy.

Suppose that equality holds in (2). Then all inequalities in the above argument must be equalities. We have to consider two cases (i)  $p > 0$ , (ii)  $p = 0$ .

Case (i): From  $1 - 1/d_j = 1 - 1/\Delta$ , we get  $d_j = \Delta$  for  $v_i v_j \in E(G)$ ,  $d_i = 1$ .

From equality in (4), we get  $d_j = \delta_1$  for  $v_i v_j \in E(G)$ ,  $d_i = 1$ .

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

Case (ii): In this case  $\delta = \delta_1 \geq 2$ . From equality in (3), for any two adjacent edges  $v_i v_j \in E(G)$ ,  $v_i v_k \in E(G)$ ,

$$\sqrt{d_i d_j} \sqrt{d_i + d_j - 2} = \sqrt{d_i d_k} \sqrt{d_i + d_k - 2}$$

i. e.,  $d_i d_j + d_j^2 - 2d_j = d_i d_k + d_k^2 - 2d_k$  as  $d_i \neq 0$

i. e.,  $(d_j - d_k)(d_i + d_j + d_k - 2) = 0$

i. e.,  $d_j = d_k$  since  $d_i + d_j + d_k > 2$ . (5)

Suppose that  $d_i = r$ . Then by (5), all vertices adjacent to the vertex  $v_i$  are of the same degree (say,  $s$ ), and all vertices adjacent to the vertex  $v_j$ ,  $v_i v_j \in E(G)$ , are of degree  $r$ . Using (5) and the fact that  $G$  is connected, it follows that each vertex of degree  $r$  is adjacent to vertices of degree  $s$ , and each vertex of degree  $s$  is adjacent to vertices of degree  $r$ . Thus  $G$  is a bipartite semiregular graph or  $G$  is a regular graph.

Conversely, let  $G$  be a  $(\Delta, 1)$ -semiregular graph. Then,  $M_1(G) = (n - p)\Delta^2 + p$ ,  $M_2^*(G) = p/\Delta + (m - p)/\Delta^2$ , and  $(n - p)\Delta = 2(m - p) + p$ . Using these relations, we get

$$[M_1(G) - 2m - p(\delta_1 - 1)] \left[ M_2^*(G) - \frac{p}{\Delta} \right] = [(n - p)\Delta^2 + 2p - 2m - p\Delta] \frac{(m - p)}{\Delta^2} = \frac{2(\Delta - 1)}{\Delta^2} (m - p)^2.$$

Hence equality holds in (2).

Let  $G$  be an  $r$ -regular graph. Then

$$\sqrt{(M_1(G) - 2m)M_2^*(G)} = \sqrt{(nr^2 - nr) \frac{m}{r^2}} = m \sqrt{\frac{2}{r} - \frac{2}{r^2}} = ABC(G)$$

since  $2m = nr$ .

Let  $G$  be a bipartite  $(r, s)$ -semiregular graph. Also, let  $k$  be the number of vertices of degree  $r$ , and  $\ell$  be the number of vertices of degree  $s$ . Then  $kr = \ell s = m$  and we have

$$\sqrt{(M_1(G) - 2m)M_2^*(G)} = \sqrt{(kr^2 + \ell s^2 - 2m)\frac{m}{rs}} = m\sqrt{\frac{1}{r} + \frac{1}{s} - \frac{2}{rs}} = ABC(G)$$

which completes the proof of Theorem 2.2.  $\square$

By setting  $p = 0$  in Theorem 2.2, we get:

**Corollary 2.3.** *With the same notation as in Theorem 2.2,*

$$ABC(G) \leq \sqrt{(M_1 - 2m)M_2^*}. \tag{6}$$

Equality in (6) holds if and only if  $G$  is regular or bipartite semiregular.

**Corollary 2.4.** [2] *With the same notation as in Theorem 2.2,*

$$ABC(G) \leq p\sqrt{1 - \frac{1}{\Delta} + \frac{m-p}{\delta_1}}\sqrt{2(\delta_1 - 1)}. \tag{7}$$

The case of equality in (7) is complicated and has been determined in [2].

### 3. Nordhaus–Gaddum–type results for ABC index

Motivated by the seminar work of Nordhaus and Gaddum [14], we report here analogous results for the ABC index. For this we need:

**Lemma 3.1.** [2] *Let  $G$  be a simple connected graph with  $m$  edges and maximal vertex degree  $\Delta$ . Then*

$$ABC(G) \geq \frac{2^{7/4}m\sqrt{\Delta - 1}}{\Delta^{3/4}(\sqrt{\Delta} + \sqrt{2})} \tag{8}$$

where equality is attained if and only if  $G \cong P_n$ .

**Theorem 3.2.** *Let  $G$  be a simple connected graph of order  $n$  with connected complement  $\bar{G}$ . Then*

$$ABC(G) + ABC(\bar{G}) \geq \frac{2^{3/4}n(n-1)\sqrt{k-1}}{k^{3/4}(\sqrt{k} + \sqrt{2})} \tag{9}$$

where  $k = \max\{\Delta, n - \delta - 1\}$ , and where  $\Delta$  and  $\delta$  are the maximal and minimal vertex degrees of  $G$ . Moreover, equality in (9) holds if and only if  $G \cong P_4$ .

*Proof.* We start by inequality (8). Let  $\bar{m}$  and  $\bar{\Delta}$  be the number of edges and maximal vertex degree in  $\bar{G}$ . Then

$$\begin{aligned} ABC(G) + ABC(\bar{G}) &\geq \frac{2^{7/4}m\sqrt{\Delta - 1}}{\Delta^{3/4}(\sqrt{\Delta} + \sqrt{2})} + \frac{2^{7/4}\bar{m}\sqrt{\bar{\Delta} - 1}}{\bar{\Delta}^{3/4}(\sqrt{\bar{\Delta}} + \sqrt{2})} \\ &= \frac{2^{3/4}2m\sqrt{\Delta - 1}}{\Delta^{3/4}(\sqrt{\Delta} + \sqrt{2})} + \frac{2^{3/4}(n(n-1) - 2m)\sqrt{n - \delta - 2}}{(n - \delta - 1)^{3/4}(\sqrt{n - \delta - 1} + \sqrt{2})}. \end{aligned} \tag{10}$$

Consider the function

$$f(x) = \frac{\sqrt{x-1}}{x^{3/4}(\sqrt{x} + \sqrt{2})}$$

for which one can easily show that it monotonically decreases in the interval  $[2, \infty]$ . Thus

$$\frac{\sqrt{\Delta-1}}{\Delta^{3/4}(\sqrt{\Delta} + \sqrt{2})} \geq \frac{\sqrt{k-1}}{k^{3/4}(\sqrt{k} + \sqrt{2})} \leq \frac{\sqrt{n-\delta-2}}{(n-\delta-1)^{3/4}(\sqrt{n-\delta-1} + \sqrt{2})} \tag{11}$$

since  $k \geq \Delta$  and  $k \geq n - \delta - 1$ . Since  $2\bar{m} = n(n-1) - 2m$ , combining the above results with (10), we arrive at (9).

It remains to examine the equality case. It is easy to check that equality in (9) holds if  $G \cong P_4$ . Suppose now that equality holds in (9). Then all inequalities in (11) must be equalities, and we get  $k = \Delta = n - 1 - \delta$ . Equality in (10) implies  $G \cong P_n$  and  $\bar{G} \cong P_n$ . Hence  $G \cong P_4$ . By this the proof of Theorem 3.2 has been completed.  $\square$

**Theorem 3.3.** Let  $G$  be a simple connected graph of order  $n$  with connected complement  $\bar{G}$ . Then

$$ABC(G) + ABC(\bar{G}) \leq (p + \bar{p}) \sqrt{\frac{n-3}{n-2}} \left(1 - \sqrt{\frac{2}{n-2}}\right) + \binom{n}{2} \sqrt{\frac{2}{k} - \frac{2}{k^2}} \tag{12}$$

where  $p, \bar{p}$  and  $\delta_1, \bar{\delta}_1$  are the number of pendent vertices and minimal non-pendent vertex degrees in  $G$  and  $\bar{G}$ , respectively, and  $k = \min\{\delta_1, \bar{\delta}_1\}$ . Equality holds in (12) if and only if  $G \cong P_4$  or  $G$  is an  $r$ -regular graph of order  $2r + 1$ .

*Proof.* We have  $\Delta \leq n - 2$ , as  $G$  and  $\bar{G}$  are connected, and hence

$$1 - \frac{1}{\Delta} \leq \frac{n-3}{n-2} \quad \text{and} \quad \frac{2}{\delta_1} - \frac{2}{\delta_1^2} \geq \frac{2(n-3)}{(n-2)^2}.$$

Bearing in mind (7), we get

$$\begin{aligned} ABC(G) &\leq p \sqrt{\frac{n-3}{n-2}} - p \sqrt{\frac{2(n-3)}{(n-2)^2}} + m \sqrt{\frac{2}{\delta_1} - \frac{2}{\delta_1^2}} \\ &= p \sqrt{\frac{n-3}{n-2}} \left(1 - \sqrt{\frac{2}{n-2}}\right) + m \sqrt{\frac{2}{\delta_1} - \frac{2}{\delta_1^2}} \end{aligned} \tag{13}$$

from which there holds

$$ABC(G) + ABC(\bar{G}) \leq (p + \bar{p}) \sqrt{\frac{n-3}{n-2}} \left(1 - \sqrt{\frac{2}{n-2}}\right) + m \sqrt{\frac{2}{\delta_1} - \frac{2}{\delta_1^2}} + \bar{m} \sqrt{\frac{2}{\bar{\delta}_1} - \frac{2}{\bar{\delta}_1^2}} \tag{14}$$

$$\leq (p + \bar{p}) \sqrt{\frac{n-3}{n-2}} \left(1 - \sqrt{\frac{2}{n-2}}\right) + (m + \bar{m}) \sqrt{\frac{2}{k} - \frac{2}{k^2}} \tag{15}$$

as  $k \leq \delta_1, \bar{\delta}_1$ .

Since  $m + \bar{m} = \binom{n}{2}$ , from (15), we get the required result (12).

We now examine the equality case.

Suppose that equality holds in (12). Then all inequalities in the above argument must be equalities. From equality in (13) we get  $\Delta = \delta_1 = n - 2$ ,  $p \neq 0$ , that is,  $G \cong P_4$  or  $G$  is isomorphic to a regular graph, by Lemma 2.4.

Equality in (14) implies that (i)  $G \cong P_4$  or  $G$  is isomorphic to a regular graph and (ii)  $\overline{G} \cong P_4$  or  $\overline{G}$  is isomorphic to a regular graph.

From equality in (15), we get  $\delta_1 = \overline{\delta}_1$ .

Using the above results, and recalling that  $\overline{P_4} \cong P_4$ , we conclude that  $G \cong P_4$  or  $G$  is isomorphic to an  $r$ -regular graph with  $n = 2r + 1$ .

Conversely, one can easily see that equality in (12) holds for the path  $P_4$  and for an  $r$ -regular graph of order  $2r + 1$ .  $\square$

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