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On atom–bond connectivity molecule structure descriptors

BORIS FURTULA[1]*, IVAN GUTMAN[1,2#] and KINKAR CH. DAS[3]

[1]*Faculty of Science, University of Kragujevac, P. O. Box 60, 34000 Kragujevac, Serbia*
[2]*State University of Novi Pazar, Novi Pazar, Serbia and* [3]*Department of Mathematics, Sungkyunkwan University, Suwon 440–746, South Korea*

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Abstract: The atom–bond connectivity index (*ABC*) is a degree-based molecular structure descriptor with well-documented chemical applications. In 2010, a distance-based new variant of this index (ABC_{GG}) was proposed. Hitherto, the relation between *ABC* and ABC_{GG} has not been analyzed. In this paper, the basic characteristics of this relation are established. In particular, *ABC* and ABC_{GG} are not correlated and both cases $ABC > ABC_{GG}$ and $ABC < ABC_{GG}$ may occur in the case of (structurally similar) molecules. However, in the case of benzenoid hydrocarbons, *ABC* always exceeds ABC_{GG}.

Keywords: atom–bond connectivity index; *ABC* index; molecular structure descriptor; molecular graph.

INTRODUCTION

One of the most prolific areas of application of graph theory in chemistry is *via* molecular structure descriptors (topological indices), namely quantities that are calculated from the molecular graphs and that are used for modeling physicochemical, pharmacological, toxicological, and other properties of the underlying chemical compounds. Several thousands such topological indices have been suggested,[1] but only a dozen or so were proved to have true applicative power. One of these is the atom–bond connectivity (*ABC*) index. It was introduced in 1998 by Estrada *et al*.,[2] but it attracted little attention. Only after the publication of a paper,[3] ten years later, did the *ABC* index rapidly gain in popularity. It was shown[2–4] that by means of the *ABC* index, it is possible to predict the thermodynamic properties of acyclic and cyclic saturated hydrocarbons, including those with large steric strain. Comparative studies[5,6] confirmed that the *ABC* index yields significantly better results than other mathematically similar molecular structure descriptors.

* Corresponding author. E-mail: furtula@kg.ac.rs
# Serbian Chemical Society member.
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The *ABC* index is defined as follows. Let *G* be a molecular graph with *n* vertices, $v_1, v_2, \ldots, v_n$. The edge of *G*, connecting the vertices v_i and v_j will be denoted by $e(i, j)$. The degree d_i of the vertex v_i is the number of the first neighbors of v_i. Then:

$$ABC = \sum_{e_{ij}} \sqrt{\frac{d_i + d_j - 2}{d_i d_j}} \tag{1}$$

with the summation going over all edges of the graph *G*.

Nowadays, the theory of the *ABC* index is well developed, and its mathematical properties have been duly examined; for details see the recent papers[7–13] and the references cited therein.

Motivated by the success of the *ABC* index, Graovac and Ghorbani[14] introduced its new variant, defined as:

$$ABC_{\mathrm{GG}} = \sum_{e_{ij}} \sqrt{\frac{n_1(e_{ij}) + n_2(e_{ij}) - 2}{n_1(e_{ij})\, n_2(e_{ij})}} \tag{2}$$

In formula (2), $n_1(e_{ij})$ is the number of vertices of *G* whose distance to the vertex v_i is smaller than the distance to the vertex v_j. Analogously, $n_2(e_{ij})$ is the number of vertices of *G* whose distance to the vertex v_j is smaller than to v_i. Vertices equidistant from both v_i and v_j are ignored. More on the numbers $n_1(e_{ij})$ and $n_2(e_{ij})$ can be found elsewhere.[15,16]

This distance-based variant of the atom–bond connectivity index was until now studied only to a limited extent.[14,17–19] Interestingly, none of the articles[14,17–19] considered the simplest and most obvious question, namely: what is the relation between the original atom–bond connectivity index *ABC*, Eq. (1), and its modified version ABC_{GG}, Eq. (2)? The aim of the present work is to provide an answer to this question.

NUMERICAL WORK

The *ABC* and ABC_{GG} indices were calculated for several classes of isomeric alkanes and cycloalkanes. In all cases studied, it was found that between these two structure descriptors there is no (either linear or any other) correlation. A typical example is presented in Fig. 1.

Not only that the two atom–bond connectivity indices are not correlated, but they also imply opposite ordering for structurally similar compounds. For instance, for 2-methylnonane, $ABC = 6.58$, $ABC_{\mathrm{GG}} = 6.49$ (thus, $ABC > ABC_{\mathrm{GG}}$), whereas for 3-methylnonane, $ABC = 6.47$, $ABC_{\mathrm{GG}} = 6.58$ (thus, $ABC < ABC_{\mathrm{GG}}$); for 2,2-dimethyloctane, $ABC = 6.84$, $ABC_{\mathrm{GG}} = 6.82$ (thus, $ABC > ABC_{\mathrm{GG}}$ but $ABC \approx ABC_{\mathrm{GG}}$), whereas for 3,3-dimethyloctane, $ABC = 6.68$, $ABC_{\mathrm{GG}} = 6.95$ (thus, $ABC < ABC_{GG}$).

Bearing in mind the good correlation properties of the original *ABC* index,[2-5] it could be concluded that there is little hope that the ABC_{GG} index would ever be found useful in chemical applications.

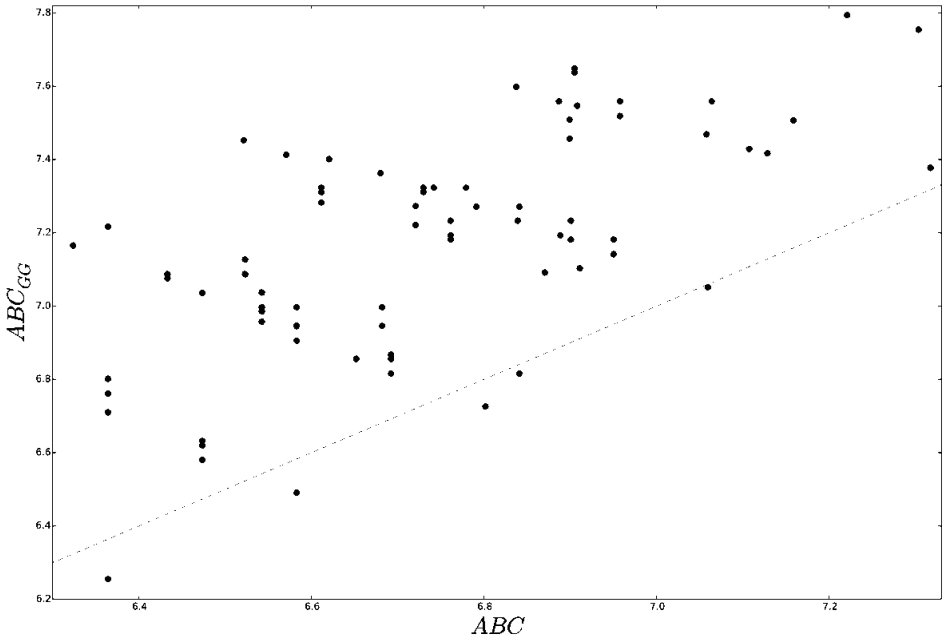

Fig. 1. Atom–bond connectivity indices of isomeric decanes plotted *versus* their ABC_{GG} values. The data points lying above (resp. below) the line, satisfy $ABC < ABC_{GG}$ (resp. $ABC > ABC_{GG}$). In the majority of cases (in this example: with only five exceptions), the ABC index is less than the ABC_{GG} index.

THE TWO ATOM–BOND CONNECTIVITY INDICES OF BENZENOID HYDROCARBONS

In this section, a few basic properties of the two ABC indices of benzenoid molecules are established. For this, the facts from the well-elaborated topological theory of benzenoid hydrocarbons were used.[20] An illustrative example is provided in Fig. 2.

Consider thus a benzenoid system with n vertices, m edges, h hexagons, n_i internal vertices, and b bay regions on its perimeter.[20] More details on parameter b can be found elsewhere.[20–22]

An edge is of (r,s)-type, if it end-vertices have degrees r and s. A benzenoid system has only vertices of degrees two and three and therefore its edges are only of (2,2)- (2,3)- and (3,3)-type. Therefore, the term:

$$\sqrt{(d_i + d_j - 2) / (d_i\, d_j)}$$

in Eq. (1) is equal to $\sqrt{2}/2$, $\sqrt{2}/2$ and $2/3$ if the edge e_{ij} is of (2,2)-, (2,3) and (3,3)-type, respectively. This implies:

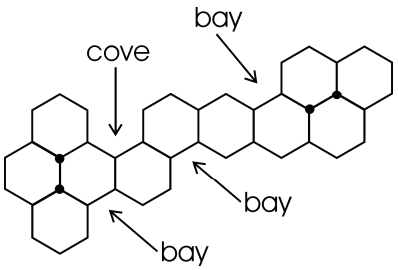

Fig. 2. A benzenoid system with $h = 11$ hexagons, $n_i = 4$ internal vertices (indicated by heavy dots), three bays and one cove, and therefore with $b = 3\times1+1\times2 = 5$ bay regions. This benzenoid system has $n = 4h + 2 - n_i = 42$ vertices and $m = 5h + 1 - n_i = 52$ edges. According to Eq. (4), the number of (3,3)-edges is $m_{33} = 11-1+4+5 = 19$.

$$ABC = \frac{\sqrt{2}}{2}m_{22} + \frac{\sqrt{2}}{2}m_{23} + \frac{2}{3}m_{33}$$

where m_{22}, m_{23} and m_{33} stand for the number of edges of the (2,2)-, (2,3)- and (3,3)-type, respectively. Since $m_{22} + m_{23} + m_{33} = m$:

$$ABC = \frac{2}{3}m_{33} + \frac{\sqrt{2}}{2}(m - m_{33}) \tag{3}$$

and m_{33} can be calculated by means of the identity:

$$m_{33} = h - 1 + n_i + b \tag{4}$$

As $2/3 < \sqrt{2}/2$, it follows from Eq. (3) that the *ABC* index is bounded as:

$$\frac{2}{3}m < ABC \leq \frac{\sqrt{2}}{2}m \tag{5}$$

The equality on the right-hand side of (5) is attained only in the case of benzene ($h = 1$).

In the case of benzenoid hydrocarbons, the quantities $n_1(e_{ij})$ and $n_2(e_{ij})$, occurring in Eq. (2), can be calculated by the method of elementary edge-cuts.[15,23,24]

An elementary edge-cut is a line segment that goes through the center of some hexagons, orthogonal to some edges, and intersects the perimeter exactly two times. The number of vertices lying on the two sides of an elementary edge-cut *C* is denoted by $n_1(C)$ and $n_2(C)$. Since $n_1(C) + n_2(C) = n$, only one among $n_1(C)$ and $n_2(C)$ requires evaluation, which is usually very simple. An illustrative example is provided in Fig. 3.

The number of edges intersected by the cut *C* will be denoted by $r(C)$, *cf.* Fig. 3. If e_{ij} is any of the edges intersected by *C*, then:

$$n_1(e_{ij}) = n_1(C) \text{ and } n_2(e_{ij}) = n_2(C)$$

For benzenoid hydrocarbons, this has the direct consequence that:

$$ABC_{GG} = \sum_C r(C)\sqrt{\frac{n_1(C) + n_2(C) - 2}{n_1(C)\,n_2(C)}}$$

holds, where the summation goes over all elementary edge-cuts. Since, in addition, for all elementary edge-cuts, $n_1(C)+n_2(C)=n$, one finally obtains:

$$ABC_{GG}=\sqrt{n-2}\sum_{C}\frac{r(C)}{\sqrt{n_1(C)n_2(C)}} \tag{6}$$

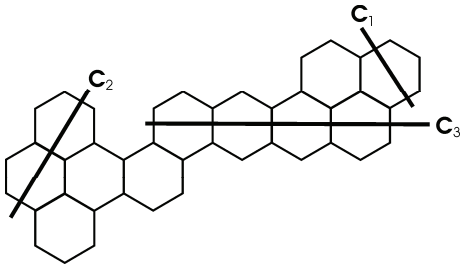

Fig. 3. Three elementary edge-cuts of the benzenoid system depicted in Fig. 2. Since this system has $n=42$ vertices, one has: $r(C_1)=2$, $n_1(C_1)=3$, $n_2(C_1)=42-3=39$, $r(C_2)=3$, $n_1(C_2)=5$, $n_2(C_2)=42-5=37$, and $r(C_3)=5$, $n_1(C_3)=15$, $n_2(C_3)=42-15=27$.

On one side of any elementary edge-cut, there are at least three vertices and at most, one-half of the total number of vertices. Therefore, $3\le n_1(C)\le n/2$, which substituted back into Eq. (6), and bearing in mind that:

$$\sum_{C}r(C)=m$$

yields the bounds:

$$\frac{2m}{n}\sqrt{n-2}\le ABC_{\mathrm{GG}}\le m\sqrt{\frac{n-2}{3(n-3)}} \tag{7}$$

Equality on both sides of (7) is attained only in the case of benzene ($h=1$).

Combining the lower bound in (5) and the upper bound in (7), one obtains:

$$\frac{ABC}{ABC_{\mathrm{GG}}}\ge\sqrt{\frac{4(n-3)}{3(n-2)}}$$

in which equality is attained only in the case of benzene ($n=6$). Thus, only in the case of benzene, do the two atom–bond connectivity indices coincide.

For all other benzenoids, $h\ge 2$, $n\ge 10$ and therefore:

$$ABC>\sqrt{\frac{4(10-3)}{3(10-2)}}\,ABC_{\mathrm{GG}}$$

i.e., $ABC>\sqrt{7/6}\,ABC_{\mathrm{GG}}$ where $\sqrt{7/6}=1.0801$. If naphthalene is excluded, then $n\ge 14$, and $ABC>\sqrt{11/9}\,ABC_{\mathrm{GG}}$ where $\sqrt{11/9}=1.1055$.

Thus, in contrast to alkanes and cycloalkanes, the atom–bond connectivity index of any benzenoid hydrocarbon is always greater than the ABC_{GG} index.

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ИЗВОД

МОЛЕКУЛСКИ СТРУКТУРНИ ДЕСКРИПТОРИ ПОВЕЗАНОСТИ ТИПА АТОМ–ВЕЗА

БОРИС ФУРТУЛА[1], ИВАН ГУТМАН[1,2] и KINKAR CH. DAS[3]

[1]Природно–математички факултет Универзитета у Крагујевцу, [2]Државни универзитет у Новом Пазару и [3]Sungkyunkwan University, Suwon, South Korea

Индекс повезаности типа атом–веза (ABC) је молекулски структурни дескриптор заснован на степенима чворова, чије су хемијске примене добро документоване. Године 2010. предложена је једна варијанта овог индекса (ABC_{GG}) заснована на растојању. До сада, релације између ABC и ABC_{GG} нису биле истраживане. У овом раду, установљене су основне карактеристике ове релације: индекси ABC и ABC_{GG} нису корелисани, и оба случаја, $ABC > ABC_{GG}$ и $ABC < ABC_{GG}$, се могу догодити код структурно сличних молекула. Међутим, у случају бензеноидних угљоводоника, ABC је увек већи од ABC_{GG}.

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