Journal of the Serbian Chemical Society
JSCS-info@shd.org.rs • www.shd.org.rs/JSCS
J. Serb. Chem. Soc. 79 (5) 557–563 (2014)
JSCS–4607
UDC 544.112+532.74:544.131:515.12
Original scientific paper

Relating the *ABC* and harmonic indices

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(Received 30 September, accepted 30 December 2013)

Abstract: The atom–bond connectivity (*ABC*) index is a much-studied molecular structure descriptor, based on the degrees of the vertices of the molecular graph. Recently, another vertex–degree-based topological index, the harmonic index (*H*), has attracted attention and gained popularity. It is shown how *ABC* and *H* are related.

Keywords: topological index; degree-based topological index; atom–bond connectivity index; *ABC* index; harmonic index.

INTRODUCTION

In contemporary theoretical chemistry, a great variety of graph-based molecular structure descriptors, so-called "topological indices", are studied and used.[1–4] Of these, about two dozens are defined in terms of vertex degrees.[5–8] Comparative testing of the vertex–degree-based topological indices[6,7] revealed that from a practical point of view, one of the best is the "atom–bond connectivity (*ABC*) index". Its applicability, especially for modeling thermochemical properties of saturated organic compounds, is nowadays well documented.[6,9,10]

The *ABC* index is defined as:

$$ABC = ABC(G) = \sum_{u,v} \sqrt{\frac{d(u)+d(v)-2}{d(u)\,d(v)}} \qquad (1)$$

where $d(u)$ denotes the degree of the vertex u, and the summation goes over all pairs of adjacent vertices of the molecular graph G. Recall[11] that the degree of a vertex is the number of its first neighbors (in the underlying graph); in graphs

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doi: 10.2298/JSC130930001G

representing organic molecules, the vertex degrees may assume only values 1, 2, 3 or 4.

Another way of expressing the *ABC* index is:[5]

$$ABC = \sum_{i \le j} \sqrt{\frac{i + j - 2}{ij}} m_{ij} \tag{2}$$

where m_{ij} denotes the number of edges connecting a vertex of degree i with a vertex of degree j.

Details of the theoretical investigation of the *ABC* index can be found in a survey,[12] recent papers,[13–18] and the references cited therein.

Using the same notation as in Eq. (1), the harmonic index is defined as:

$$H = H(G) = \sum_{u,v} \frac{2}{d(u) + d(v)} \tag{3}$$

and, in analogy, Eq. (2) can be written as:[5]

$$H = \sum_{i \le j} \frac{2}{i + j} m_{ij} \tag{4}$$

Although this quantity was first mentioning in a mathematical paper[19] from 1987, it did not attract the attention of scholars until quite recently. On the other hand, in the last few years, a remarkably large number of studies of the properties of the harmonic index have appeared,[20–28] amongst them some by two of the present authors.[20,21,24] The chemical applicability of the harmonic index was also recently investigated.[6,7]

In view of the great current research activity on the *ABC* and harmonic indices, and in view of the mathematical similarity of Eqs. (2) and (4), it could be of some interest to search for relations between them. This task is accomplished in the two subsequent sections.

RELATIONS BETWEEN *THE ABC* AND HARMONIC INDICES – GENERAL GRAPHS

In order to establish relations between the two considered topological indices, bearing in mind Eqs. (2) and (4), an auxiliary function $Q = Q(x, y)$ is introduced:

$$Q(x, y) = \frac{\sqrt{\frac{x + y - 2}{xy}}}{\frac{2}{x + y}} = \frac{x + y}{2} \sqrt{\frac{x + y - 2}{xy}} \tag{5}$$

As the variables x and y pertain to vertex degrees, for any connected graph G with n vertices, they must satisfy the condition $1 \le x \le y \le n - 1$. In addition, it

cannot be $x = y = 1$ (except in the trivial case $n = 2$, which is ignored), *i.e.*, y must be ≥ 2.

By direct calculation, one obtains:

$$\frac{\partial Q(x,y)}{\partial y} = \frac{x(y+2)+(y^2-x^2)+y(y-2)}{4y\sqrt{xy(x+y-2)}}$$

that evidently is positive-valued for all $y \geq 2$. Thus, $Q(x,y)$ is a monotonically increasing function in the variable *y*. Consequently, its minimal value is either $Q(1,2)$ or $Q(2,2)$, and its maximal value is $Q(x,n-1)$ for some *x*, which still needs to be determined.

Since:

$$Q(1,2) = \frac{3}{2\sqrt{2}} \approx 1.061$$

and:

$$Q(2,2) = \sqrt{2} \approx 1.414$$

it is concluded that *Q* is minimal for $x = 1, y = 2$.

The first derivative of $Q(x,n-1)$ is found to be:

$$\frac{\partial Q(x,n-1)}{\partial x} = \frac{2x^2+(n-3)x-(n-1)(n-3)}{4x\sqrt{(n-1)x(x+n-3)}}$$

A detailed analysis shows that for $n = 3$ and $n = 4$, the function $Q(x,n-1)$ monotonically increases and, therefore, its greatest value is $Q(n-1,n-1)$. For $n \geq 5$, this function has a minimum in the interval $(1,n-1)$ and, therefore, the greatest value of $Q(x,n-1)$ is either $Q(1,n-1)$ or $Q(n-1,n-1)$. As:

$$Q(1,n-1) = \frac{n}{2}\sqrt{\frac{n-2}{n-1}}$$

and

$$Q(n-1,n-1) = \sqrt{2n-4}$$

by direct checking one finds that for $n \leq 6$ the greatest value of the function *Q* is $Q(n-1,n-1)$, whereas for $n \geq 7$ its greatest value is $Q(1,n-1)$.

Return now to the topological indices *ABC* and *H*, Eqs. (1) and (3). Let *G* be a graph with *n* vertices. An edge of *G* is said to be of the (i, j)- type if its end--vertices have degrees *i* and *j*.

Bearing in mind Eqs. (2) and (4) and the Form (5) chosen for the function *Q*, it is seen that the ratio $ABC(G)/H(G)$ will be minimal if all edges of *G* are of the (1,2)-type. In connected graphs, this is only possible if $n = 3$ and then *G* is

just the molecular graph P_3 of propane. Thus, the first relation, valid for all graphs, is obtained:

$$\frac{ABC(G)}{H(G)} \geq Q(1,2) = \frac{3}{2\sqrt{2}} \tag{6}$$

with equality (for connected graphs) if and only if $G = P_3$.

In the same manner, it could be concluded that for $n \leq 6$, the ratio $ABC(G) / H(G)$ will be maximal if all edges of G are of the $(n-1, n-1)$-type, whereas for $n \geq 7$, all edges should be of the $(1, n-1)$-type.

Therefore, if $n \leq 6$, then:

$$\frac{ABC(G)}{H(G)} \leq Q(n-1, n-1) = \sqrt{2n-4} \tag{7}$$

with equality if and only if G is a complete graph.[11]

If $n \geq 7$, then:

$$\frac{ABC(G)}{H(G)} \leq Q(1, n-1) = \frac{n}{2}\sqrt{\frac{n-2}{n-1}} \tag{8}$$

with equality if and only if G is a star graph.[11]

Summarizing the relations (6)–(8), the first main result can be stated:

Proposition 1. Let G be any graph with n vertices, $n > 2$. Then:

$$\gamma_1 H(G) \leq ABC(G) \leq \gamma_2 H(G) \text{ and } \delta_1 ABC(G) \leq H(G) \leq \delta_2 ABC(G)$$

where:

$$\gamma_1 = \frac{3}{2\sqrt{2}},\ \gamma_2 = \sqrt{2}, 2, \sqrt{6}, 2\sqrt{2} \text{ and } \frac{n}{2}\sqrt{\frac{n-2}{n-1}}$$

for $n = 3, 4, 5, 6$, and $n \geq 7$, respectively, and:

$$\delta_1 = \frac{1}{\gamma_2} \text{ and } \delta_2 = \frac{1}{\gamma_1}.$$

Equality cases are specified at Eqs. (6)–(8).

RELATIONS BETWEEN *ABC* AND HARMONIC INDICES – MOLECULAR GRAPHS

In the case of molecular graphs, the analysis of the relation between the ABC and harmonic indices is much simpler, thanks to the fact that these graphs may have only 9 different types of edges. The respective Q-values are given in Table I.

Using the values from Table I and an analogous, yet simpler, reasoning as in the preceding section, second main result is straightforwardly deduced:

Proposition 2. Let G be any molecular graph with n vertices, $n > 2$. Then:

$$Q(1,2)H(G) \le ABC(G) \le Q(4,4)H(G) \text{ and}$$
$$\frac{1}{Q(4,4)}ABC(G) \le H(G) \le \frac{1}{Q(1,2)}ABC(G)$$

where the values of $Q(i, j)$ are given in Table I. The equality $ABC(G) = Q(1,2)H(G)$ occurs if and only if G is the molecular graph of propane. In the case of ordinary molecular graphs, the equality $ABC(G) = Q(4,4)H(G)$ is not possible, but could be satisfied if G is the graph representation of a diamond-like nanostructure.[29,30]

For benzenoid systems, in which only (2,2)-, (2,3)- and (3,3)-type edges occur (*i.e.*, in Eqs. (2) and (4) the only non-zero multipliers are m_{22}, m_{23}, m_{33}),[5,31–33] the following special case of Proposition 2 holds:

Proposition 3. Let G be the molecular graph of a benzenoid system. Then:

$$Q(2,2)H(G) \le ABC(G) \le Q(3,3)H(G) \text{ and}$$
$$\frac{1}{Q(3,3)}ABC(G) \le H(G) \le \frac{1}{Q(2,2)}ABC(G)$$

where the values of $Q(i, j)$ are given in Table I. The equality $ABC(G) = Q(2,2)H(G)$ occurs if and only if G is the molecular graph of benzene. The equality $ABC(G) = Q(3,3)H(G)$ occurs in the cases of nanotubes and nanotoruses, as well as fullerenes.[29,30]

TABLE I. The value of the auxiliary function Q, Eq. (5), for all possible edge-types that may occur in molecular graphs; i, j are the degrees of the end-vertices of the respective edge

i, j	$Q(i, j)$	i, j	$Q(i, j)$
1,2	1.061	2,4	2.121
1,3	1.633	3,3	2.000
1,4	2.165	3,4	2.259
2,2	1.414	4,4	2.449
2,3	1.768		

Acknowledgement. The second author was supported by the National Natural Science Foundation of China (Nos. 11001129 and 11226289) and the Fundamental Research Funds for the Nanjing University of Aeronautics and Astronautics (No. NS2013075). The third author was supported by the National Natural Science Foundation of China (No. 11201227), the Natural Science Foundation of Jiangsu Province (No. BK20131357), and a China Postdoctoral Science Foundation Funded Project (No. 2013M530253).

ИЗВОД

ВЕЗЕ ИЗМЕЂУ *ABC* И ХАРМОНИЈСКОГ ИНДЕКСА

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Индекс повезаности атом–веза (*atom–bond connectivity index*, *ABC*) је један од највише проучаваних молекулских структурних дескриптора заснованих на степенима чворова молекулског графа. Недавно је један други такав тополошки индекс – хармонијски индекс *H* – привукао пажњу и добио на значају. У раду налазимо везе између *ABC* и *H*.

(Примљено 30. септембра, прихваћено 30. децембра 2013)

REFERENCES

1. J. Devillers, A. T. Balaban (Eds.), *Topological Indices and Related Descriptors in QSAR and QSPR*, Gordon & Breach, Amsterdam,1999
2. R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Wiley-VCH, Weinheim, Germany, 2000
3. R. Todeschini, V. Consonni, *Molecular Descriptors for Chemoinformatics*, *Vols. 1* and *2*, Wiley-VCH, Weinheim, Germany, 2009
4. I. Gutman, B. Furtula (Eds.), *Novel Molecular Structure Descriptors – Theory and Applications*, Vols. 1 and 2, Univ. Kragujevac, Kragujevac, 2010
5. I. Gutman, B. Furtula, *J. Serb. Chem. Soc.* **77** (2012) 1031
6. I. Gutman, J. Tošović, *J. Serb. Chem. Soc.* **78** (2013) 805
7. B. Furtula, I. Gutman, M. Dehmer, *Appl. Math. Comput.* **219** (2013) 8973
8. I. Gutman, *Croat. Chem. Acta* **86** (2013) 351
9. E. Estrada, *Chem. Phys. Lett.* **463** (2008) 422
10. I. Gutman, J. Tošović, S. Radenković, S. Marković, *Indian J. Chem., A* **51** (2012) 690
11. I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer, Berlin, 1986
12. I. Gutman, B. Furtula, M. B. Ahmadi, S. A. Hosseini, P. Salehi Nowbandegani, M. Zarrinderakht, *Filomat* **27** (2013) 1075
13. I. Gutman, B. Furtula, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 131
14. I. Gutman, B. Furtula, M. Ivanović, *MATCH Commun. Math. Comput. Chem.* **67** (2012) 467
15. W. Lin, X. Lin, T. Gao, X. Wu, *MATCH Commun. Math. Comput. Chem.* **69** (2013) 549
16. M. B. Ahmadi, S. A. Hosseini, P. Salehi Nowbandegani, *MATCH Commun. Math. Comput. Chem.* **69** (2013) 559
17. M. B. Ahmadi, S. A. Hosseini, M. Zarrinderakht, *MATCH Commun. Math. Comput. Chem.* **69** (2013) 565
18. S. A. Hosseini, M. B. Ahmadi, I. Gutman, *MATCH Commun. Math. Comput. Chem.* **71** (2014) 5
19. S. Fajtlowicz, *Congr. Numer.* **60** (1987) 187
20. L. Zhong, *Appl. Math. Lett.* **25** (2012) 561
21. L. Zhong, *Ars Combin.* **104** (2012) 261
22. J. Liu, Q. Zhang, *Util. Math.* **88** (2012) 281
23. X. Xu, *Appl. Math. Sci.* **41** (2012) 2013
24. L. Zhong, K. Xu, *Util. Math.* **90** (2013) 23

25. Y. Zhu, R. Chang, X. Wei, *Ars Comb*. **110** (2013) 97
26. R. Wu, Z. Tang, H. Deng, *Util. Math.* **91** (2013) 65
27. H. Deng, S. Balachandran, S. K. Ayyaswamy, Y. B. Venkatakrishnan, *Discr. Appl. Math.* **161** (2013) 2740
28. R. Wu, Z. Tang, H. Deng, *Filomat* **27** (2013) 51
29. M. V. Diudea, C. L. Nagy, *Periodic Nanostructures*, Springer, Amsterdam, 2007
30. M. V. Diudea, *Nanomolecules and Nanostructures*, Univ. Kragujevac, Kragujevac, 2010
31. J. Rada, R. Cruz, I. Gutman, *Chem. Phys. Lett.* **572** (2013) 154
32. R. Cruz, H. Giraldo, J. Rada, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 501
33. J. Rada, R. Cruz, I. Gutman, *MATCH Commun. Math. Comput. Chem*. **72** (2014) 125.