Electronic Journal of Mathematics
www.shahindp.com/locate/ejm

Electron. J. Math. **5** (2023) 1–7
DOI: 10.47443/ejm.2022.039

Research Article

Atom-bond sum-connectivity index of unicyclic graphs and some applications

Akbar Ali[1], Ivan Gutman[2,*], Izudin Redžepović[2,3]

[1]*Department of Mathematics, College of Science, University of Ha'il, Ha'il, Saudi Arabia*
[2]*Faculty of Science, University of Kragujevac, Kragujevac, Serbia*
[3]*Department of Natural Sciences and Mathematics, State University of Novi Pazar, Novi Pazar, Serbia*

(Received: 23 September 2022. Received in revised form: 10 October 2022. Accepted: 11 October 2022. Published online: 14 October 2022.)

Abstract

The atom-bond sum-connectivity (ABS) index is a recently introduced variant of three earlier much studied graph-based molecular descriptors: connectivity (Randić), atom-bond connectivity, and sum-connectivity indices. In this paper, the graphs with minimum, second-minimum, maximum, and second-maximum values of the ABS index are determined over the class of connected unicyclic graphs with a fixed order. Possible chemical applications of the ABS index are also investigated on particular sets of chemical graphs.

Keywords: connectivity index; atom-bond connectivity index; sum-connectivity index; atom-bond sum-connectivity index; unicyclic graph.

2020 Mathematics Subject Classification: 05C07, 05C09, 05C38, 05C92.

1. Introduction

Throughout the present paper, the graphs considered are finite and connected. For graph theoretical terminology and notation used without being defined, we refer the readers to the books [5, 6, 27].

The *connectivity index* of a graph G is defined as (see [22, 23])

$$R(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u\, d_v}}\,,$$

where $E(G)$ is the set of edges of G, uv represents the edge connecting the vertices u and v, and d_u denotes the degree of the vertex u. By the majority of scholars, $R(G)$ is called *Randić index* [12, 15, 24].

Estrada et al. [9] introduced a modified version of the connectivity index and referred it to as the *atom-bond connectivity index*. It is defined as

$$ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u\, d_v}}\,.$$

Another variant of the connectivity index was put forwarded by Zhou and Trinajstić [28] under the name *sum-connectivity index*. It is defined as

$$\chi(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u + d_v}}\,.$$

Details concerning the mathematical aspects of the connectivity, atom-bond connectivity, and sum-connectivity indices together with their applications can be found in [1, 3, 8, 12, 14, 15, 18, 23, 24] and the references cited therein.

A modified version of the atom-bond connectivity index, utilizing the core idea of the sum-connectivity index and named *atom-bond sum-connectivity (ABS) index*, was recently put forward in [2]. The ABS index is defined as

$$ABS(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u + d_v}} = \sum_{uv\in E(G)} \sqrt{1 - \frac{2}{d_u + d_v}}\,.$$

The ABS index is a particular case of the so-called t-index, devised and investigated by Tang et al. [26]. It needs to be remarked that the t-index was considered in [26] for several choices of the parameters, but none of these pertained to the ABS index.

In [2] were characterized the graphs having extreme values of the ABS index among (molecular) trees and general graphs with a fixed order. In the present paper, we report analogous results for unicyclic graphs and give some possible chemical applications of the ABS index.

*Corresponding author (gutman@kg.ac.rs).

2. Atom-bond sum-connectivity index of unicyclic graphs

For a vertex u in a graph G, denote by $N(u)$ the set of all those vertices of G that are adjacent with u.

Lemma 2.1. *Let v_1v_2 be an edge of the graph G such that it does not lie on a triangle, and $d_{v_1} \geq d_{v_2} \geq 2$. Construct the graph $G^\star$ by removing from G all edges of the set $\{v_2u : u \in N(v_2) \setminus \{v_1\}\}$, and adding all the new edges of the set $\{v_1u : u \in N(v_2) \setminus \{v_1\}\}$. Then $ABS(G^\star) > ABS(G)$.*

Proof. In this proof, by d_x we mean the degree of the vertex $x \in V(G) = V(G^\star)$ in G, not in $G^\star$. By using the definition of the ABS index one has

$$\begin{aligned} ABS(G) - ABS(G^\star) &= \sum_{u \in N(v_2)\setminus\{v_1\}} \left(\sqrt{1 - \frac{2}{d_{v_2} + d_u}} - \sqrt{1 - \frac{2}{d_{v_1} + d_{v_2} + d_u - 1}} \right) \\ &+ \sum_{w \in N(v_1)\setminus\{v_2\}} \left(\sqrt{1 - \frac{2}{d_{v_1} + d_w}} - \sqrt{1 - \frac{2}{d_{v_1} + d_{v_2} + d_w - 1}} \right). \end{aligned} \tag{1}$$

Since $d_{v_1} \geq d_{v_2} \geq 2$ and the function F defined by

$$F(x_1, x_2) = \sqrt{1 - \frac{2}{x_1 + x_2}}$$

is strictly increasing in x_1 as well as in x_2 for $x_1 \geq 1$ and $x_2 \geq 1$, the required inequality follows from (1). □

Among the several direct consequences of Lemma 2.1, we mention the following two.

Corollary 2.1 (see [2])**.** *For every fixed integer n greater than 3, the star S_n is the only graph possessing the maximum ABS index in the class of all trees of order n.*

Corollary 2.2. *If n is a fixed integer greater than 3, and G is a graph with the maximum ABS index in the class of all unicyclic graphs of order n, then G has $n-3$ vertices of degree 1; see the graph depicted in Figure 1.*

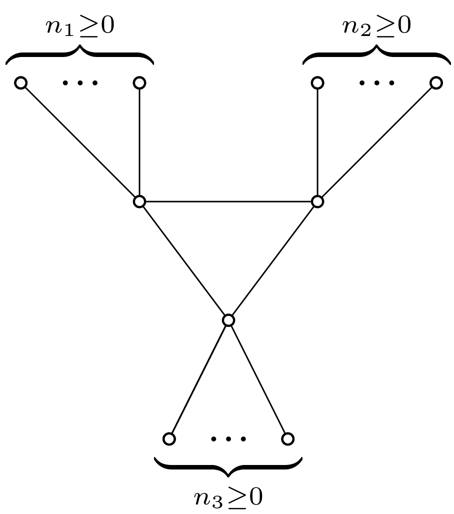

Figure 1: The unicyclic graph of order n referred in Corollary 2.2, obtained by attaching vertices of degree 1 to the triangle C_3. Here, $n_3 \geq n_2 \geq n_1 \geq 0$ and $n_1 + n_2 + n_3 = n - 3$.

An n-vertex graph is a graph with n vertices. A vertex of degree 1 is known as a pendent vertex. For every fixed integer n greater than 3, let S_n^+ be the n-vertex graph obtained by attaching $n-3$ pendent vertices to one vertex of the triangle C_3. Note that S_n^+ is the graph depicted in Figure 1 for which $n_1 = n_2 = 0$ and $n_3 = n - 3$.

Proposition 2.1. *Among all unicyclic graphs of order $n > 3$, the graph S_n^+ has the maximum ABS index, equal to*

$$(n-3)\sqrt{\frac{n-2}{n}} + 2\sqrt{\frac{n-1}{n+1}} + \frac{1}{\sqrt{2}}\,.$$

Proof. Let G^* be the graph with the maximum ABS index among all unicyclic graphs of order n. By Corollary 2.2, G^* has $n-3$ vertices of degree 1. Therefore, G^* must be a graph shown in Figure 1. Since $n_3 \geq n_2 \geq n_1 \geq 0$ and $n_1+n_2+n_3 = n-3$, it holds that $\lfloor (n-3)/3 \rfloor \geq n_3 \geq n_2 \geq n_1 \geq 0$. By utilizing the definition of the ABS index, we have

$$ABS(G^*) = \sum_{i=1}^{3} n_i \sqrt{1 - \frac{2}{n_i+3}} + \sum_{1 \leq i < j \leq 3} \sqrt{1 - \frac{2}{n_i+n_j+4}} \,. \tag{2}$$

Equation (2) can be written in terms of n, n_1, and n_2 as

$$\begin{aligned} ABS(G^*) &= (n-n_1-n_2-3)\sqrt{1-\frac{2}{n-n_1-n_2}} + n_1\sqrt{1-\frac{2}{n_1+3}} + n_2\sqrt{1-\frac{2}{n_2+3}} \\ &+ \sqrt{1-\frac{2}{n-n_2+1}} + \sqrt{1-\frac{2}{n-n_1+1}} + \sqrt{1-\frac{2}{n_1+n_2+4}} \,. \end{aligned} \tag{3}$$

Let φ be the bivariate function defined by

$$\begin{aligned} \varphi(x_1,x_2) &= (n-x_1-x_2-3)\sqrt{1-\frac{2}{n-x_1-x_2}} + x_1\sqrt{1-\frac{2}{x_1+3}} + x_2\sqrt{1-\frac{2}{x_2+3}} \\ &+ \sqrt{1-\frac{2}{n-x_2+1}} + \sqrt{1-\frac{2}{n-x_1+1}} + \sqrt{1-\frac{2}{x_1+x_2+4}} \,, \end{aligned}$$

where x_1 and x_2 are real numbers satisfying $\lfloor (n-3)/3 \rfloor \geq x_2 \geq x_1 \geq 0$. We note that

$$\begin{aligned} \frac{\partial \varphi}{\partial x_2} &= -\frac{n-x_1-x_2-3}{\sqrt{1-\frac{2}{n-x_1-x_2}}\,(n-x_1-x_2)^2} - \sqrt{1-\frac{2}{n-x_1-x_2}} - \frac{1}{\sqrt{1-\frac{2}{n-x_2+1}}\,(n-x_2+1)^2} \\ &+ \sqrt{1-\frac{2}{x_2+3}} + \frac{x_2}{(x_2+3)^2\sqrt{1-\frac{2}{x_2+3}}} + \frac{1}{(x_1+x_2+4)^2\sqrt{1-\frac{2}{x_1+x_2+4}}} \,. \end{aligned} \tag{4}$$

Setting $y_1 = x_2+3$ and $y_2 = n-x_1-x_2$ in (4) yields

$$\begin{aligned} \frac{\partial \varphi}{\partial x_2} &= \frac{1}{(x_1+y_1+1)^2\sqrt{1-\frac{2}{x_1+y_1+1}}} - \frac{1}{(x_1+y_2+1)^2\sqrt{1-\frac{2}{x_1+y_2+1}}} + \frac{y_1-3}{y_1^2\sqrt{1-\frac{2}{y_1}}} \qquad (5) \\ &+ \sqrt{1-\frac{2}{y_1}} - \sqrt{1-\frac{2}{y_2}} - \frac{y_2-3}{y_2^2\sqrt{1-\frac{2}{y_2}}} \\ &= \psi(x_1,y_1) - \psi(x_1,y_2) \qquad (6) \end{aligned}$$

where

$$\psi(x_1,z) = \frac{1}{(x_1+z+1)^2\sqrt{1-\frac{2}{x_1+z+1}}} + \frac{z-3}{z^2\sqrt{1-\frac{2}{z}}} + \sqrt{1-\frac{2}{z}} \,.$$

We also have

$$\begin{aligned} \frac{\partial \psi}{\partial z} &= \frac{(-2x_1-2z+1)\sqrt{1-\frac{2}{x_1+z+1}}}{((x_1+z)^2-1)^2} + \frac{6z-9}{(z-2)^{3/2}z^{5/2}} - \frac{1}{(z-2)^{3/2}z^{3/2}} \\ &= f(x_1,z) + \frac{6z-9}{(z-2)^{3/2}z^{5/2}} - \frac{1}{(z-2)^{3/2}z^{3/2}} \end{aligned} \tag{7}$$

where

$$f(x_1,z) = \frac{(-2x_1-2z+1)\sqrt{1-\frac{2}{x_1+z+1}}}{((x_1+z)^2-1)^2} \,.$$

If $z \geq y_1$, then $z \geq 3$ (because $y_1 = x_2+3$ and $x_2 \geq x_1 \geq 0$) and thence

$$\frac{\partial f}{\partial x_1} = \frac{3\big(2x_1^2+2x_1(2z-1)+2z(z-1)+1\big)}{\sqrt{\frac{x_1+z-1}{x_1+z+1}}\,(x_1+z-1)^2(x_1+z+1)^4} > 0 \,.$$

This implies $f(x_1, z) \geq f(0, z)$ for $z \geq y_1$, and hence from (7) it follows that

$$\frac{\partial \psi}{\partial z} \geq \frac{(-2z+1)\sqrt{1-\frac{2}{z+1}}}{(z^2-1)^2} + \frac{6z-9}{(z-2)^{3/2}z^{5/2}} - \frac{1}{(z-2)^{3/2}z^{3/2}} > 0 \tag{8}$$

for $z \geq y_1$ (that is, for $z \geq 3$). Since $\lfloor (n-3)/3 \rfloor \geq x_2 \geq x_1 \geq 0$, it holds that

$$y_2 = n - x_1 - x_2 \geq x_2 + 3 = y_1$$

which gives $\psi(x_1, y_2) \geq \psi(x_1, y_1)$. Thus, from (6) it follows that the function φ is decreasing in x_2. Similarly, by symmetry, φ is decreasing in x_1. Therefore, $\varphi(x_1, x_2) \leq \varphi(0, 0)$. Thus, from (3) it follows that

$$ABS(G^*) \leq (n-3)\sqrt{\frac{n-2}{n}} + 2\sqrt{\frac{n-1}{n+1}} + \frac{1}{\sqrt{2}} = ABS(S_n^+) . \qquad \square$$

For every fixed integer n greater than 4, let S_n^{++} be the n-vertex graph obtained by attaching $n-4$ pendent vertices to one vertex of the triangle C_3, and attaching a pendent vertex to another vertex of C_3. Note that S_n^{++} is the graph depicted in Figure 1 for which $n_1 = 0$, $n_2 = 1$, and $n_3 = n-4$.

In an analogous manner as Proposition 2.1 we can prove:

Proposition 2.2. *Among all unicyclic graphs of order $n > 4$, the graph S_n^{++} has the second-maximum ABS index, equal to*

$$(n-4)\sqrt{\frac{n-3}{n-1}} + \sqrt{\frac{n-1}{n+1}} + \sqrt{\frac{n-2}{n}} + \sqrt{\frac{3}{5}} + \frac{1}{\sqrt{2}} .$$

A path $u_1 \cdots u_r$ in a graph G is said to be a pendent path if $\min\{d_{u_1}, d_{u_r}\} = 1$, $\max\{d_{u_1}, d_{u_r}\} \geq 3$, and $d_{u_i} = 2$ for $2 \leq i \leq r-1$. A vertex of a graph with degree at least 3 is called a branching vertex. Certainly, every pendent path has exactly one branching vertex. We say that two pendent paths in a graph are adjacent if they have a common branching vertex.

Lemma 2.2 (see [2]). *If a graph G has at least one pair of adjacent pendent paths, then there exists at least one graph G' containing no pair of adjacent pendent paths such that $ABS(G) > ABS(G')$.*

Proposition 2.3. *For every fixed integer $n \geq 3$, among all unicyclic graphs of order n, the cycle C_n is the only graph possessing the minimum ABS index, equal to $n/\sqrt{2}$.*

Proof. Suppose that G is a unicyclic graph of order n with the minimum ABS index. By Lemma 2.2, G has no pair of adjacent pendent paths, which means that the maximum degree of G is at most 3 and every vertex of maximum degree lies on the cycle of G. We claim that G does not have any pendent path. Contrarily, suppose that $vv_1 \cdots v_t$ is a pendent path of G where the vertex v lies on the cycle of G. Let u, v_1, and w be the neighbors of v. If G' is the graph obtained from G by deleting the edge vu and inserting a new edge $v_t u$, then

$$ABS(G) - ABS(G') = \sqrt{1-\frac{2}{d_u+3}} + \sqrt{1-\frac{2}{d_w+3}} - \sqrt{1-\frac{2}{d_u+2}} - \sqrt{1-\frac{2}{d_w+2}}$$
$$+ \begin{cases} \dfrac{1}{\sqrt{2}} - \sqrt{\dfrac{3}{5}} & \text{if } t = 1, \\[2ex] \dfrac{1}{\sqrt{3}} + \sqrt{\dfrac{3}{5}} - \sqrt{2} & \text{if } t > 1. \end{cases}$$

Here, d_u and d_w represent degrees of the vertices u and w (respectively) in G, not in G'. Since the maximum degree of G is 3, it holds that

$$\sqrt{1-\frac{2}{d_x+3}} - \sqrt{1-\frac{2}{d_x+2}} \geq \sqrt{\frac{2}{3}} - \sqrt{\frac{3}{5}}$$

for $x \in \{u, w\}$ and thus $ABS(G) - ABS(G') > 0$, which contradicts the minimality of $ABS(G)$. Therefore, G does not have any pendent path, which means that $G \cong C_n$. $\square$

In an analogous manner we can prove the next result.

Proposition 2.4. *For every fixed integer $n > 4$, among all unicyclic graph of order n, every graph having exactly one pendent path such that the unique pendent path has length at least 2 possesses the second-minimum value of the ABS index, equal to*

$$\frac{n-4}{\sqrt{2}} + 3\sqrt{\frac{3}{5}} + \frac{1}{\sqrt{3}} .$$

3. Chemical applicability of the ABS index

	ABS	R	χ	ABC
ABS	1.0000	0.9975	0.9915	0.9811
R		1.0000	0.9977	0.9700
χ			1.0000	0.9550
ABC				1.0000

Table 1: The absolute values of the correlation coefficients between some indices.

Correlation coefficients among ABS, R, ABC, and χ indices are presented in Table 1, in the case of octane isomers. From these values we may conclude that the ABS index may predict equally well the properties of molecules that can be predicted by any of the three indices. To test this, we have correlated our indices with the experimental physico-chemical properties of octane isomers. Complete experimental data are available at

https://web.archive.org/web/20180912171255if_/http://www.moleculardescriptors.eu/index.htm

for the following thirteen physico-chemical properties: boiling point, heat capacity at P constant, heat capacity at T constant, density, entropy, enthalpy of vaporization, enthalpy of formation, standard enthalpy of vaporization, standard enthalpy of formation, total surface area, acentric factor, molar volume, octanol-water partition coefficient. The absolute value of the correlation coefficient between each of these thirteen properties and ABS index is calculated and those greater than 0.8 are listed in Table 2. The absolute values of the correlation coefficients between these (six) properties and the three indices R, χ, ABC, are also listed in the same table.

	ABS	R	χ	ABC
Boiling point	**0.8356**	0.8208	0.8023	0.8323
Entropy	0.8847	0.9058	0.9230	0.8146
Enthalpy of vaporization	**0.9402**	0.9361	0.9318	0.9151
Standard enthalpy of vaporization	0.9545	0.9582	0.9612	0.9170
Enthalpy of formation	**0.8602**	0.8505	0.8316	0.8497
Acentric factor	0.8801	0.9042	0.9299	0.8076

Table 2: The absolute values of the correlation coefficients between six properties of octane isomers and our indices.

From Table 2, it is observed that the ABS index performs somewhat better than the ABC index for the six listed properties. Also, the ABS index outperforms all the considered indices for boiling point, enthalpy of vaporization, and enthalpy of formation.

In Table 3 the percentage of degeneracy of ABS, R, χ, and ABC indices for several sets of chemical trees is presented. As one may see, the ABS index shows degeneracy levels comparable with other indices. Such modest discriminative potential is in accordance with the degeneracy of other degree-based graph invariants [25].

n	# of isomers	ABS	R	χ	ABC
10	75	37.33	34.67	37.33	41.33
11	159	50.94	47.17	50.94	54.09
12	355	65.07	61.13	65.07	66.48
13	802	75.94	72.07	75.94	76.43
14	1858	84.61	81.05	84.50	84.28
15	4347	90.20	87.53	90.25	90.11

Table 3: The percentage of degeneracy of ABS, R, χ, and ABC indices in the case of chemical trees.

Another important feature of a topological index is its structure sensitivity [21]. In Figure 2 the percentage of structure sensitivity of ABS, R, χ, and ABC indices in the case of decane isomers is depicted. As can be seen, the ABS index shows comparable percentage of structure sensitivity with other investigated indices. This finding indicates that the ABS index can successfully describe subtle modifications within molecular structure.

4. Concluding remarks

In this paper, we found the graphs extremal with respect to the ABS index over the class of all unicyclic graphs of a fixed order. We have also investigated the chemical applicability of the ABS index on the set of octane isomers and found that

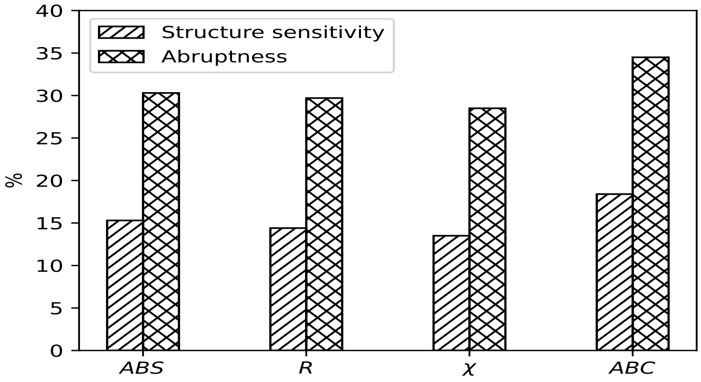

Figure 2: Structure sensitivity of ABS, R, χ, and ABC indices in the case of decane isomers.

it is strongly correlated with the connectivity, atom-bond connectivity, and sum-connectivity indices. This indicates that the ABS index can be used to predict properties of molecules equally well (or better than) as by the earlier connectivity indices. Moreover, the ABS index performs slightly better than the aforementioned indices in predicting certain chemical properties of octane isomers; when comparing ABS and ABC indices, the ABS index outperforms the ABC index in six properties.

For a possible future work towards the study of the ABS index, consider its general version:

$$ABS_\alpha(G) = \sum_{uv \in E(G)} \left(\frac{d_u + d_v - 2}{d_u + d_v} \right)^\alpha ,$$

where α is a real number and G does not have any component isomorphic to the path of order 2 when $\alpha < 0$. Consider the closed interval $[-5, 5]$ and the set of octane isomers together with the six chemical properties mentioned in Table 2. Is there any value of α (different from $1/2$) in the considered interval for which ABS_α predicts at least one of the mentioned property better than the ordinary ABS index? It is a question similar to the one addressed in [10] for the case of the general ABC index.

Another direction for a possible future work towards the study of the ABS index is concerned with extremal results. Such results concerning the minimum values of the ABS index seem to be interesting because similar results involving the ABC index are not easy to obtain in many cases. For example, the problem of finding trees having the minimum ABC index over the class of all trees of a fixed order was perhaps one of the much-investigated and hard problems in chemical graph theory in the last decade (for example, see [1]) and was recently settled in [7, 13]. On the other hand, surprisingly, the corresponding problem for the ABS index was rather easy [2]. (It was proved in [2] that the star and path graphs are the only extremal trees with respect to the ABS index among all trees of a given order; this indicates that the ABS index may also be useful within the theory of branching in molecules and graphs, for example see [4].) Finding trees having the minimum ABC index over the class of a fixed number of pendent vertices was another challenging problem, which was addressed in several papers (for example, see [11, 16, 17, 19]) and was finally solved by Mohar in [20]. Thus, it would be interesting to find a solution to the following problem.

Problem 4.1. *Find trees having the minimum ABS index over the class of a fixed number of pendent vertices.*

Acknowledgements

Akbar Ali is partially supported by the Scientific Research Deanship, University of Ha'il, Saudi Arabia, through project numbers RG-22 002 and RG-22 005. Izudin Redžepović gratefully acknowledges the financial support of the Serbian Ministry of Education, Science and Technological Development (Grant No. 451-03-68/2022-14/200122) and the State University of Novi Pazar.

References

[1] A. Ali, K. C. Das, D. Dimitrov, B. Furtula, Atom-bond connectivity index of graphs: a review over extremal results and bounds, *Discrete Math. Lett.* **5** (2021) 68–93.
[2] A. Ali, B. Furtula, I. Redžepović, I. Gutman, Atom-bond sum-connectivity index, *J. Math. Chem.*, In press, DOI: 10.1007/s10910-022-01403-1.
[3] A. Ali, L. Zhong, I. Gutman, Harmonic index and its generalization: extremal results and bounds, *MATCH Commun. Math. Comput. Chem.* **81** (2019) 249–311.
[4] S. H. Bertz, Branching in graphs and molecules, *Discrete Appl. Math.* **19** (1988) 65–83.
[5] J. A. Bondy, U. S. R. Murty, *Graph Theory*, Springer, London, 2008.

[6] G. Chartrand, L. Lesniak, P. Zhang, *Graphs & Digraphs*, CRC Press, Boca Raton, 2016.

[7] D. Dimitrov, Z. Du, Complete characterization of the minimal-ABC trees, *arXiv*:2110.14712 [math.CO], (2022).

[8] E. Estrada, Atom-bond connectivity and the energetic of branched alkanes, *Chem. Phys. Lett.* **463** (2008) 422–425.

[9] E. Estrada, L. Torres, L. Rodríguez, I. Gutman, An atom-bond connectivity index: modelling the enthalpy of formation of alkanes, *Indian J. Chem. Sec. A* **37** (1998) 849–855.

[10] B. Furtula, A. Graovac, D. Vukičević, Augmented Zagreb index, *J. Math. Chem.* **48** (2010) 370–380.

[11] M. Goubko, C. Magnant, P. Salehi Nowbandegani, I. Gutman, ABC index of trees with fixed number of leaves, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 697–702.

[12] I. Gutman, B. Furtula (Eds.), *Recent Results in the Theory of Randić Index*, Univ. Kragujevac, Kragujevac, 2008.

[13] S. A. Hosseini, B. Mohar, M. B. Ahmadi, The evolution of the structure of ABC-minimal trees, *J. Combin. Theory Ser. B* **152** (2022) 415–452.

[14] X. Li, I. Gutman, *Mathematical Aspects of Randić-Type Molecular Structure Descriptors*, Univ. Kragujevac, Kragujevac, 2006.

[15] X. Li, Y. Shi, A survey on the Randić index, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 127–156.

[16] W. Lin, J. Chen, C. Ma, Y. Zhang, J. Chen, D. Zhang, J. Fei, On trees with minimal ABC index among trees with given number of leaves, *MATCH Commun. Math. Comput. Chem.* **76** (2016) 131–140.

[17] W. Lin, P. Li, J. Chen, C. Ma, Y. Zhang, D. Zhang, On the minimal ABC index of trees with k leaves, *Discrete Appl. Math.* **217** (2017) 622–627

[18] B. Lučić, S. Nikolić, N. Trinajstić, B. Zhou, S. I. Turk, Sum-connectivity index, In: I. Gutman, B. Furtula (Eds.), *Novel Molecular Structure Descriptors – Theory and Applications I*, Univ. Kragujevac, Kragujevac, 2010, 101–136.

[19] C. Magnant, P. S. Nowbandegani, I. Gutman, Which tree has the smallest ABC index among trees with k leaves?, *Discrete Appl. Math.* **194** (2015) 143–146.

[20] B. Mohar, The structure of ABCŰminimal trees with given number of leaves, *MATCH Commun. Math. Comput. Chem.* **79** (2018) 415–430.

[21] M. Rakić, B. Furtula, A novel method for measuring the structure sensitivity of molecular descriptors, *J. Chemom.* **33** (2019) #e3138.

[22] M. Randić, M. On characterization of molecular branching, *J. Amer. Chem. Soc.* **97** (1975) 6609–6615.

[23] M. Randić, The connectivity index 25 years after, *J. Mol. Graph. Model.* **20** (2001) 19–35.

[24] M. Randić, On history of the Randić index and emerging hostility toward chemical graph theory, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 5–124.

[25] I. Redžepović, Chemical applicability of Sombor indices, *J. Serb. Chem. Soc.* **86** (2021) 445–457.

[26] Y. Tang, D. B. West, B. Zhou, Extremal problems for degree-based topological indices, *Discrete Appl. Math.* **203** (2016) 134–143.

[27] S. Wagner, H. Wang, *Introduction to Chemical Graph Theory*, CRC Press, Boca Raton, 2018.

[28] B. Zhou, N. Trinajstić, On a novel connectivity index, *J. Math. Chem.* **46** (2009) 1252–1270.