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Research Article

On the atom-bond sum-connectivity spectral radius of trees

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Abstract

The atom-bond sum-connectivity (ABS) matrix of a graph G with n vertices is the square matrix of order n whose (i,j)-entry is equal to $\sqrt{(d_i+d_j-2)/(d_i+d_j)}$ if the i-th vertex and the j-th vertex of G are adjacent, and 0 otherwise, where d_i is the degree of the i-th vertex of G. The ABS spectral radius of G is the largest eigenvalue of the ABS matrix of G, which is denoted by $\lambda_{ABS}(G)$. In this paper, the chemical importance of the ABS spectral radius is investigated and it is found that this new spectral parameter is useful in predicting certain physicochemical properties of molecules with an accuracy higher than the atom-bond sum-connectivity index. Also, for any tree T_n with $n \geq 5$ vertices, it is proved that $\lambda_{ABS}(P_n) \leq \lambda_{ABS}(T_n) \leq \lambda_{ABS}(S_n)$, with equality in the left (respectively, right) inequality if and only if T_n is isomorphic to the path P_n (respectively, the star S_n).

Keywords: ABS matrix; ABS spectral radius; tree.

2020 Mathematics Subject Classification: 05C05, 05C09, 05C35, 05C92.

1. Introduction

Establishing mathematical models for the connections between molecular structures and physicochemical properties of chemical compounds is a frequently used approach to study the quantitative structure-activity relationship and quantitative structure-property relationship [11]. For this purpose, many kinds of molecular-graph-based structure descriptors were proposed, including degree-based topological indices [19], distance-based topological indices [3], and spectral-based topological indices [12,18,22,26]. Matrix representation of a (molecular) graph preserves more structural information than a single-valued topological index; hence, a trend in mathematical chemistry is the matricalization of topological indices (weighted adjacency matrix [9]) and use of their eigenvalues to predict the physicochemical properties of molecules.

Let G be a graph with vertex set $V(G) = \{v_1, v_2, ..., v_n\}$ and edge set $E(G)$. The atom-bond connectivity index (ABC index for short) of G, introduced by Estrada et al. [15], is defined as

$$ABC(G) = \sum_{v_iv_j \in E(G)} \sqrt{\frac{d_i + d_j - 2}{d_i d_j}},$$

where d_i is the degree of a vertex $v_i \in V(G)$. This index has an excellent correlation with the heat of formation of alkanes [15]. A topological approach was developed on the basis of the ABC index to explain the differences in the energy of linear and branched alkanes, both qualitatively and quantitatively [13]. After that, extensive research was conducted on this index from mathematical and chemical perspectives; for instance, see [10] and references cited therein.

In 2017, Estrada [14] proposed the ABC matrix and studied the mathematical properties of the eigenvalues of this matrix (called ABC eigenvalues), such as ABC energy and ABC Estrada index. Chen [4] obtained several basic properties for the ABC eigenvalues, and gave bounds on the ABC energy. Gao and Shao [16] proved that the star S_n has the minimum ABC energy among all trees with n vertices, which solves Chen's conjecture [4]. Ghorbani [17] established some new bounds for the ABC energy. On the other hand, the study of ABC spectral radius (that is, the largest eigenvalue of the ABC matrix) is an interesting topic. Chen [5] characterized the trees with the maximum or minimum ABC spectral radius. Li and Wang [20] determined the unicyclic graphs with the maximum or minimum ABC spectral radius. Yuan et al. [24] determined the unicyclic graphs with the first four largest values of the ABC spectral radius. Yuan and Du [23] determined the bicyclic graphs with the first two maximum values of the ABC spectral radius. Chen [6] characterized the (connected) graphs and (connected) triangle-free graphs having the maximum or first two minimum value(s) of the ABC spectral radius.

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Inspired by the ABC index, Ali et al. [1] recently proposed a new degree-based topological index, called the atom-bond sum-connectivity index (ABS index for short), which is defined as

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

The ABS matrix of a graph G is defined to be the square matrix $\mathcal{ABS}(G) = (\omega_{ij})$ whose entries are given as

$$\omega_{ij} = \begin{cases} \sqrt{\dfrac{d_i + d_j - 2}{d_i + d_j}} & \text{if } v_iv_j \in E(G), \\ 0 & \text{otherwise.} \end{cases}$$

Naturally, the properties of the eigenvalues of the ABS matrix have attracted our attention. The largest eigenvalue of the ABS matrix of G is called the ABS spectral radius, denoted by $\lambda_{ABS}(G)$. In this paper, we compare the prediction power of the ABS spectral radius and the ABC spectral radius with some physical properties of octane isomers. We find that the ABS spectral radius is a good topological index in forecasting the acentric factor (AcenFac, for short) and entropy. Both the spectral radii are good in predicting the SNar and HNar of octane isomers. Since chemical graphs of octane isomers are trees, we study the extremal problem for the ABS spectral radius of trees, and prove that for any tree T_n with $n \geq 5$ vertices,

$$\lambda_{ABS}(P_n) \leq \lambda_{ABS}(T_n) \leq \lambda_{ABS}(S_n)$$

with equality in the left (respectively, right) inequality if and only if T_n is isomorphic to the path graph P_n (respectively, the star graph S_n).

2. Chemical applicability of the ABS spectral radius

In this section, we study the relationship between the acentric factor (respectively, entropy, SNar, HNar) of the octane isomers and the ABC spectral radius or the ABS spectral radius. The complete experimental data on the physicochemical properties of octane isomers is available at

https://web.archive.org/web/20170712072219/http://www.moleculardescriptors.eu/dataset/c8.rar.

Chemical graphs of octane isomers are trees with 8 vertices and the maximum degree less than or equal to 4, see Table A4 of [8]. The ABC spectral radius (λ_{ABC}) and ABS spectral radius (λ_{ABS}) of octane isomers are shown in Table 2.1. The correlation coefficient between the acentric factor, entropy, SNar, HNar of octane isomers and ABC spectral radius and ABS spectral radius are shown in Table 2.2.

Ali et al. [2] found that the values of the correlation coefficient between AcenFac and entropy of octane isomers and ABS index (respectively, ABC index) are approximately equal to -0.8801 and -0.8847 (respectively, -0.8076 and -0.8146). By Table 2.2, the values of the correlation coefficient between AcenFac and entropy of octane isomers and ABS spectral radius (respectively, ABC spectral radius) are approximately equal to -0.9765 and -0.9158 (respectively, -0.9301 and -0.9064). Thus, the ABS and ABC spectral radii are better than the ABS and ABC indices in predicting AcenFac and entropy of octane isomers. Table 2.2 also shows that the ABS spectral radius is a good predictor for AcenFac, entropy, SNar, and HNar of octane isomers. Scatter plots between AcenFac (respectively, entropy, SNar, HNar) of octane isomers and the ABS spectral radius are shown in Figure 2.1. Also, we have

$$\begin{aligned} AcenFac &= -0.2579\lambda_{ABS} + 0.7431, \\ Entropy &= -30.82\lambda_{ABS} + 154.1, \\ SNar &= -0.2343\lambda_{ABS} + 7.233 \\ HNar &= -0.6208\lambda_{ABS} + 2.389. \end{aligned}$$

An obvious question is how the two structural descriptors ABC and ABS spectral radii are related for the case of trees. Through testing chemical trees (trees with maximum degree less than or equal to 4) with 15 vertices, we find that the correlation between these two spectral radii is not considerably high (it is about 0.8524), as shown in Figure 2.2. This explains why the introduction of the ABS spectral radius as a spectral prediction parameter is reasonable in mathematical chemistry. At the same time, a question that may be of interest arises as follows:

Question 2.1. *Let $\mathcal{T}_n$ be the number of trees with n vertices. Let τ_n be the number of those trees with n vertices for which the inequality $\lambda_{ABS} > \lambda_{ABC}$ holds. What is $\lim_{n\to\infty} \frac{\tau_n}{\mathcal{T}_n}$?*

Table 2.1: Experimental data of AcenFac, entropy, SNar, HNar, λ_{ABC} and λ_{ABS} for octane isomers.

Molecule	AcentFac	Entropy	SNar	HNar	λ_{ABC}	λ_{ABS}
octane	0.3979	111.67	4.159	1.6	1.3289	1.3076
2-methyl-heptane	0.3779	109.84	3.871	1.5	1.4541	1.4102
3-methyl-heptane	0.3710	111.26	3.871	1.5	1.4462	1.4520
4-methyl-heptane	0.3715	109.32	3.871	1.5	1.4543	1.4677
3-ethyl-hexane	0.3625	109.43	3.871	1.5	1.4344	1.4922
2,2-dimethyl-hexane	0.3394	103.42	3.466	1.391	1.7000	1.6354
2,3-dimethyl-hexane	0.3482	108.02	3.584	1.412	1.5386	1.5568
2,4-dimethyl-hexane	0.3442	106.98	3.584	1.412	1.5228	1.5195
2,5-dimethyl-hexane	0.3568	105.72	3.584	1.412	1.5082	1.4687
3,3-dimethyl-hexane	0.3226	104.74	3.466	1.391	1.6594	1.6714
3,4-dimethyl-hexane	0.3403	106.59	3.584	1.412	1.5229	1.5744
2-methyl-3-ethyl-pentane	0.3324	106.06	3.584	1.412	1.5231	1.5802
3-methyl-3-ethyl-pentane	0.3069	101.48	3.466	1.391	1.6143	1.6922
2,2,3-trimethyl-pentane	0.3008	101.31	3.178	1.315	1.7251	1.7262
2,2,4-trimethyl-pentane	0.3054	104.09	3.178	1.315	1.7234	1.6733
2,3,3-trimethyl-pentane	0.2932	102.06	3.178	1.315	1.6973	1.7372
2,3,4-trimethyl-pentane	0.3174	102.39	3.296	1.333	1.5933	1.6261
2,2,3,3-tetramethylbutane	0.2553	93.06	2.773	1.231	1.8371	1.8428

Table 2.2: The correlation coefficient of AcenFac, entropy, SNar and HNar of octane isomers with λ_{ABC} and λ_{ABS}.

	AcentFac	Entropy	SNar	HNar
λ_{ABC}	-0.9301	-0.9064	-0.9551	-0.9396
λ_{ABS}	-0.9765	-0.9158	-0.9442	-0.9367

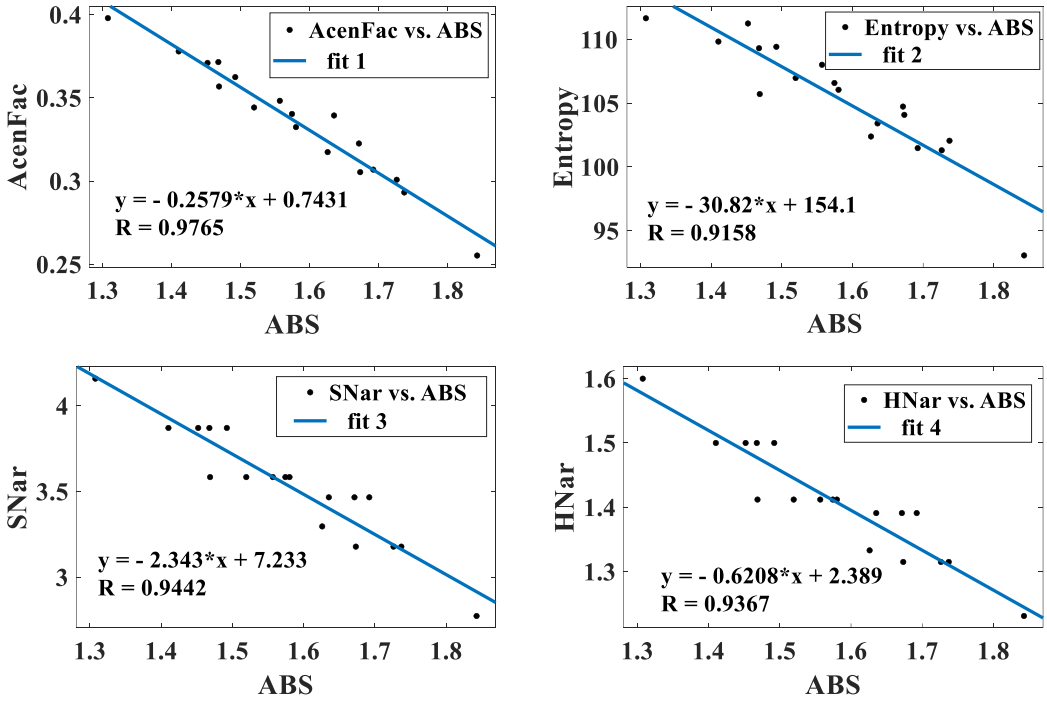

Figure 2.1: Scatter plots between AcenFac (respectively, entropy, SNar, HNar) of octane isomers and ABS spectral radius.

3. An extremal problem for the ABS spectral radius of trees

Note that chemical graphs of octane isomers are trees. In this section, we study the bounds of ABS spectral radius of trees with $n \geq 5$. Let $\lambda_A(G)$ be the spectral radius (the largest eigenvalue of the adjacency matrix $\mathcal{A}(G)$) of a graph G. Let $\lambda(M)$ be the largest eigenvalue of the matrix M.

Lemma 3.1 (see [8]). *If T_n is a tree with $n \geq 3$ vertices, then*

$$2\cos\frac{\pi}{n+1} \leq \lambda_A(T_n) \leq \sqrt{n-1},$$

with equality in the left (respectively,, right) inequality if and only if $T \cong P_n$ (respectively, $T \cong S_n$).

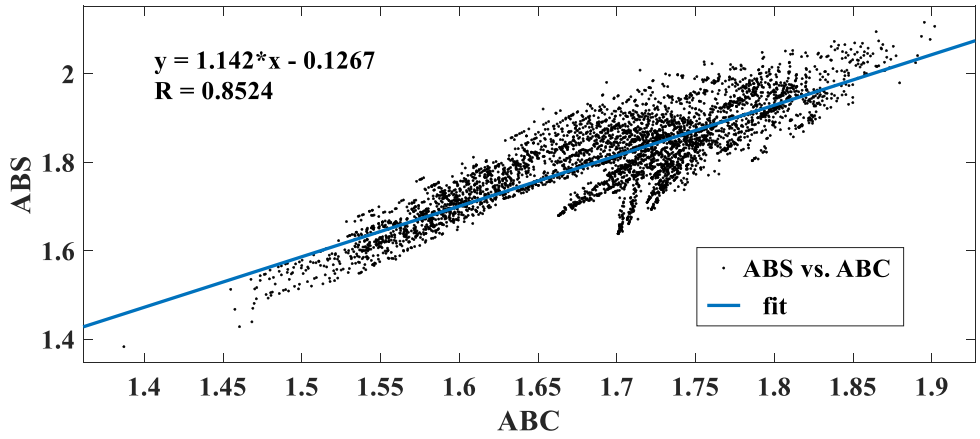

Figure 2.2: Scatter plots between the ABC spectral radius and the ABS spectral radius of chemical trees with 15 vertices.

Lemma 3.2 (see [7]). *Suppose that $A = (a_{i,j})$ and $B = (b_{i,j})$ are two $n \times n$ nonnegative symmetric matrices. If $A \geq B$, i.e., $a_{i,j} \geq b_{i,j}$ for all i, j, then $\lambda(A) \geq \lambda(B)$. Furthermore, if B is irreducible and $A \neq B$, then $\lambda(A) > \lambda(B)$.*

Lemma 3.3 (see [7]). *If M' is a principal sub-matrix of a real symmetric matrix M, then $\lambda(M) \geq \lambda(M')$.*

Theorem 3.1. *Let T_n be a tree with $n \geq 5$ vertices. Then*

$$\lambda_{ABS}(P_n) \leq \lambda_{ABS}(T_n) \leq \lambda_{ABS}(S_n),$$

with equality in the left (respectively, right) inequality if and only if $T_n \cong P_n$ (respectively, $T_n \cong S_n$).

Proof. We first prove the upper bound. Suppose that $\mathcal{ABS}(T_n) = (\omega_{ij})_{n\times n}$. For every edge v_iv_j in T_n, we assume that $\max\{d_i + d_j\} = d_1 + d_2 \leq n$. Let $f(x, y) = \sqrt{\frac{x+y-2}{x+y}} = \sqrt{1 - \frac{2}{x+y}}$. Then $f(x, y)$ is an increasing function with respect to $x + y$. Thus,

$$\omega_{ij} = f(d_i, d_j) \leq f(d_1, d_2) \leq \sqrt{1 - \frac{2}{n}},$$

which yields that

$$\mathcal{ABS}(T_n) \leq f(d_1, d_2)\mathcal{A}(T_n) \leq \sqrt{1 - \frac{2}{n}}\mathcal{A}(T_n).$$

By Lemmas 3.1 and 3.2, we have

$$\lambda_{ABS}(T_n) \leq \sqrt{1 - \frac{2}{n}}\lambda_A(T_n) \leq \sqrt{\frac{(n-1)(n-2)}{n}} = \lambda_{ABS}(S_n).$$

Now, we prove the lower bound. Let C_n denote the cycle on n vertices. We note that

$$\mathcal{ABS}(P_n) < \mathcal{ABS}(C_n) = \frac{\sqrt{2}}{2}\mathcal{A}(C_n).$$

By Lemma 3.2, we have

$$\lambda_{ABS}(P_n) < \frac{\sqrt{2}}{2}\lambda_A(C_n) \leq \sqrt{2}.$$

Consider all trees with n vertices, for $n = 5, 6, 7, 8, 9$, depicted in Table A4 [8]. Here, we have

$$\lambda_{ABS}(P_n) < \lambda_{ABS}(T_n)$$

for $5 \leq n \leq 8$ and $T_n \ncong P_n$. For $n = 9$, Table 3.1 gives the ABS spectral radius of these trees. Let T_9^* be the principal sub-matrix of order 9 of T_n with $n \geq 10$. We assume that T_9^* and T_9 have the same adjacency matrix, where $T_9 \in \{T^{48}, T^{48}, \ldots, T^{93}\}$. By Lemmas 3.2 and 3.3, we have

$$\lambda_{ABS}(T_n) \geq \lambda_{ABS}(T_9^*) \geq \lambda_{ABS}(T_9) > \sqrt{2} > \lambda_{ABS}(P_n)$$

for $n \geq 10$. In summary, we have

$$\lambda_{ABS}(T_n) \geq \lambda_{ABS}(P_n)$$

with equality if and only if $T_n \cong P_n$. This completes the proof. □

Table 3.1: The spectral radius of $A(T^i)$ and $ABC(T^i)$ for trees T^i with 9 vertices for $48 \leq i \leq 94$.

Trees	λ_A	λ_{ABS}	Trees	λ_A	λ_{ABS}	Trees	λ_A	λ_{ABS}
T^{48}	2.8284	2.4944	T^{64}	2.2638	1.7719	T^{80}	2.1358	1.6133
T^{49}	2.6762	2.3086	T^{65}	2.2470	1.7597	T^{81}	2.3897	1.7682
T^{50}	2.5396	2.1371	T^{66}	2.2361	1.7533	T^{82}	2.1120	1.5919
T^{51}	2.5243	2.1161	T^{67}	2.2361	1.7526	T^{83}	2.0840	1.5578
T^{52}	2.4972	2.1038	T^{68}	2.2164	1.7356	T^{84}	2.0840	1.5642
T^{53}	2.4495	2.0157	T^{69}	2.1940	1.6919	T^{85}	2.0743	1.5241
T^{54}	2.3968	1.9495	T^{70}	2.1679	1.6861	T^{86}	2.0608	1.5381
T^{55}	2.3761	1.9369	T^{71}	2.1358	1.6514	T^{87}	2.0356	1.5004
T^{56}	2.3268	1.8962	T^{72}	2.2361	1.7321	T^{88}	2.0000	1.4597
T^{57}	2.3761	1.9207	T^{73}	2.2059	1.7118	T^{89}	2.0529	1.5192
T^{58}	2.3467	1.9049	T^{74}	2.1753	1.6641	T^{90}	2.0421	1.5041
T^{59}	2.3344	1.8674	T^{75}	2.1753	1.6917	T^{91}	2.0153	1.4808
T^{60}	2.3073	1.8776	T^{76}	2.1646	1.6520	T^{92}	2.0000	1.4598
T^{61}	2.2361	1.7701	T^{77}	2.1646	1.6774	T^{93}	1.9616	1.4173
T^{62}	2.2882	1.8057	T^{78}	2.1169	1.6017	T^{94}	1.9021	1.3295
T^{63}	2.2552	1.7738	T^{79}	2.1169	1.6377	-	-	-

Remark 3.1. *Since* $f(x,y) = \sqrt{1-\frac{2}{x+y}}$ *is a concave function with respect to the variable* x*, the results of [21, 25] cannot be used to obtain the lower bound (given in Theorem 3.1) on the* ABS *spectral radius of trees.*

4. Conclusion

In this paper, we examined the ABC spectral radius and the ABS spectral radius for predicting the acentric factor, entropy, SNar, and HNar of octane isomers. We found that the ABS spectral radius can help significantly to predict these properties of octane isomers, which confirms its suitability in the Quantitative Structure-Property Relationship analysis. It turned out that the ABS and ABC spectral radii are better than the ABS and ABC indices in predicting AcenFac and entropy of octane isomers, see Table 2 in [2] and Table 2.2. Also, the ability of the ABS spectral radius in distinguishing tree structures is stronger than that of the spectral radius and ABS index, see Table 3 in [2], Table 2.1, and Table 3.1; that is, the degeneracy of the ABS spectral radius is relatively low. Since the chemical graphs of octane isomers are trees, we studied an extremal problem for the ABS spectral radius of trees and proved that for a tree T_n with $n \geq 5$ vertices, the inequality

$$\lambda_{ABS}(P_n) \leq \lambda_{ABS}(T_n) \leq \lambda_{ABS}(S_n)$$

holds with equality in the left (respectively, right) inequality if and only if $T_n \cong P_n$ (respectively, $T_n \cong S_n$). Solving the following general problems about the ABS spectral radius seems to be interesting:

Problem 4.1. *Characterize the chemical trees with the maximum or minimum* ABS *spectral radius.*

Problem 4.2. *For a given class of graphs, characterize the graphs with the maximum or minimum* ABS *spectral radius.*

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References

[1] A. Ali, B. Furtula, I. Redžepović, I. Gutman, Atom-bond sum-connectivity index, *J. Math. Chem.* **60** (2022) 2081–2093.
[2] A. Ali, I. Gutman, I. Redžepović, Atom-bond sum-connectivity index of unicyclic graphs and some applications, *Electron. J. Math.* **5** (2023) 1–7.
[3] M. Arockiaraj, S. Klavžar, S. Mushtaq, K. Balasubramanian, Distance-based topological indices of nanosheets, nanotubes and nanotori of SiO_2, *J. Math. Chem.* **57** (2019) 343–369.
[4] X. Chen, On ABC eigenvalues and ABC energy, *Linear Algebra Appl.* **544** (2018) 141–157.
[5] X. Chen, On extremality of ABC spectral radius of a tree, *Linear Algebra Appl.* **564** (2019) 159–169.
[6] X. Chen, A note on the ABC spectral radius of graphs, *Linear Multilinear Algebra* **70** (2022) 775–786.
[7] D. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs*, Academic Press, New York, 1980.
[8] D. Cvetković, P. Rowlinson, S. Simić, *An Introduction to the Theory of Graph Spectra*, Cambridge University Press, New York, 2010.
[9] K. Das, I. Gutman, I. Milovanović, E. Milovanović, B. Furtula, Degree-based energies of graphs, *Linear Algebra Appl.* **554** (2018) 185–204.
[10] D. Dimitrov, Z. Du, The ABC Index Conundrum's Complete Solution, *MATCH Commun. Math. Comput. Chem.* **91** (2024) 5–38.
[11] M. V. Diudea, *QSPR/QSAR Studies by Molecular Descriptors*, Nova, Huntington, 2001.
[12] E. Estrada, Characterization of 3D molecular structure, *Chem. Phys. Lett.* **319** (2000) 713–718.

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

[14] E. Estrada, The ABC matrix, *J. Math. Chem.* **55** (2017) 1021–1033.

[15] 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.

[16] Y. Gao, Y. Shao, The minimum ABC energy of trees, *Linear Algebra Appl.* **577** (2019) 186–203.

[17] M. Ghorbani, X. Li, M. Hakimi-Nezhaad, J. Wang, Bounds on the ABC spectral radius and ABC energy of graphs, *Linear Algebra Appl.* **598** (2020) 145–164.

[18] I. Gutman, The energy of a graph, *Ber. Math.-Stat. Sekt. Forschungszent. Graz* **103** (1978) 1–22.

[19] I. Gutman, Degree-based topological indices, *Croat. Chem. Acta* **86** (2013) 351–361.

[20] X. Li, J. Wang, On the ABC spectra radius of unicyclic graphs, *Linear Algebra Appl.* **596** (2020) 71–81.

[21] X. Li, Z. Wang, Trees with extremal spectral radius of weighted adjacency matrices among trees weighted by degree-based indices, *Linear Algebra Appl.* **620** (2021) 61–75.

[22] L. Lovász, J. Pelikán, On the eigenvalues of trees, *Period. Math. Hung.* **3** (1973) 175–182.

[23] Y. Yuan, Z. Du, The first two maximum ABC spectral radii of bicyclic graphs, *Linear Algebra Appl.* **615** (2021) 28–41.

[24] Y. Yuan, B. Zhou, Z. Du, On large ABC spectral radii of unicyclic graphs, *Discrete Appl. Math.* **298** (2021) 56–65.

[25] R. Zheng, X. Guan, X. Jin, Extremal trees and unicyclic graphs with respect to spectral radius of weighted adjacency matrices with property P^*, *J. Appl. Math. Comput.* **69** (2023) 2573–2594.

[26] R. Zheng, P. Su, X. Jin, Arithmetic-geometric matrix of graphs and its applications, *Appl. Math. Comput.* **442** (2023) #127764.