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Research article

On the general atom-bond sum-connectivity index

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Abstract: This paper is concerned with a generalization of the atom-bond sum-connectivity (ABS) index, devised recently in [A. Ali, B. Furtula, I. Redžepović, I. Gutman, Atom-bond sum-connectivity index, *J. Math. Chem.*, **60** (2022), 2081–2093]. For a connected graph G with an order greater than 2, the general atom-bond sum-connectivity index is represented as $ABS_\gamma(G)$ and is defined as the sum of the quantities $(1-2(d_x+d_y)^{-1})^\gamma$ over all edges xy of the graph G, where d_x and d_y represent the degrees of the vertices x and y of G, respectively, and γ is any real number. For $-10 \le \gamma \le 10$, the significance of ABS_γ is examined on the data set of octane isomers for predicting six selected physicochemical properties of the mentioned compounds; promising results are obtained when the approximated value of γ belongs to the set $\{-3, 1, 3\}$. The effect of the addition of an edge between two non-adjacent vertices of a graph under ABS_γ is also investigated. Moreover, the graphs possessing the maximum value of ABS_γ, with $\gamma > 0$, are characterized from the set of all connected graphs of a fixed order and a fixed (i) vertex connectivity not greater than a given number or (ii) matching number.

Keywords: topological index; chemical graph theory; atom-bond sum-connectivity; general atom-bond sum-connectivity
Mathematics Subject Classification: 05C07, 05C90

1. Introduction

A property of a graph that is preserved by the graph isomorphism is called a graph invariant [9]. Topological indices are widely used to refer to real-valued graph invariants. We refer the reader to the books [5, 9, 23] for (chemical-)graph-theory terminology and notations.

Among the much-investigated and applied topological indices, the connectivity index [10] (also known as the Randić index, which was invented in [19] under the name branching index) has secured a prominent place. According to [10], the connectivity index is presumed to be the topological index that has been predominantly examined, both theoretically and practically. The following number associated with a graph G is the connectivity index of G:

$$R(G) = \sum_{st\in E(G)} \frac{1}{\sqrt{d_s d_t}},$$

where $E(G)$ represents the edge set of G and d_v denotes the degree of a vertex v in G. (If two or more graphs are being considered at a time, then we use $d_v(G)$ to represent the degree of v in G to avoid confusion.) The survey papers [13, 18], books [11, 12] and related articles referred therein provide further information regarding the investigation of the connectivity index.

The popularity of the connectivity index has led to the introduction of several variants of this index in the literature. Among the extensively researched variants of the connectivity index are the sum-connectivity (SC) index [24] and the atom-bond connectivity (ABC) index [6,7] (see also [20,21]), which are defined by

$$SC(G) = \sum_{st\in E(G)} \frac{1}{\sqrt{d_s + d_t}}$$

and

$$ABC(G) = \sum_{st\in E(G)} \sqrt{\frac{d_s + d_t - 2}{d_s d_t}},$$

respectively. A new version of the ABC index, known as the atom-bond sum-connectivity (ABS) index, was developed in [2] using the basic concept of the SC index. For a graph G, the ABS index is defined as follows:

$$ABS(G) = \sum_{st\in E(G)} \sqrt{1 - \frac{2}{d_s + d_t}}.$$

Some extremal problems regarding the ABS index of (molecular) tree graphs and general graphs were solved in [2]. In [3], not only was an extremal problem regarding the ABS index for unicyclic graphs solved, but also chemical applications of the ABS index were reported. The trees, with a given number of vertices of degree 1 and with a given order, having the least ABS index were independently investigated in preprints [4, 16]; the maximal version of this problem was solved recently in [17].

The general ABS index [3] is defined by

$$ABS_\gamma(G) = \sum_{st\in E(G)} \left(1 - \frac{2}{d_s + d_t}\right)^{\gamma},$$

where γ may take any real number, provided that if $\gamma < 0$, then the graph G satisfies the inequality $d_s + d_t > 2$ for every $st \in E(G)$. We make a note here that the general ABS index (and hence the ABS index) is a particular form of a more general topological index of this kind, as introduced in [22]. For a recent study on the general ABS index, we refer the reader to [1].

In the next section, the significance of ABS_γ is examined on the data set of octane isomers for predicting six selected physicochemical properties of the mentioned compounds for $-10 \le \gamma \le 10$; promising results are obtained when the approximated value of γ belongs to the set $\{-3, 1, 3\}$. Section 3 is devoted to investigating the effect of the addition of an edge in a non-complete graph under ABS_γ, where a non-complete graph is a graph different from the complete graph. In Section 4, we characterize the graphs possessing the maximum value of ABS_γ, with $\gamma > 0$, in the set of all connected graphs of a fixed order and a fixed (i) vertex connectivity not greater than a given number or (ii) matching number.

2. Chemical usefulness of the general ABS index

In [1], the chemical applicability of the ABS_γ, with the constraint $-10 \leq \gamma \leq 10$, was tested on the data set of 25 benzenoid hydrocarbons for predicting their enthalpy of formation; it was concluded that the predictive ability of ABS_γ for the considered property of the examined hydrocarbons is comparable to other existing general indices of this kind. In the present section, the significance of ABS_γ is examined on the data set of octane isomers for predicting six selected physicochemical properties of the mentioned compounds for $-10 \leq \gamma \leq 10$. These six properties are the following: enthalpy of vaporization, boiling point, acentric factor, enthalpy of formation, entropy and standard enthalpy of vaporization. The experimental data for these selected properties can be found in [15].

The positive values of the correlation r (between the selected properties of the considered compounds and ABS_γ), with $\gamma \in [-10, 10]$, are depicted in Figures 1–6. The maximum positive values of the correlation r (between the selected properties of the considered compounds and ABS_γ), with $\gamma \in [-10, 10]$ and with $\gamma \in [-3, 3]$, are given in Tables 1 and 2, respectively.

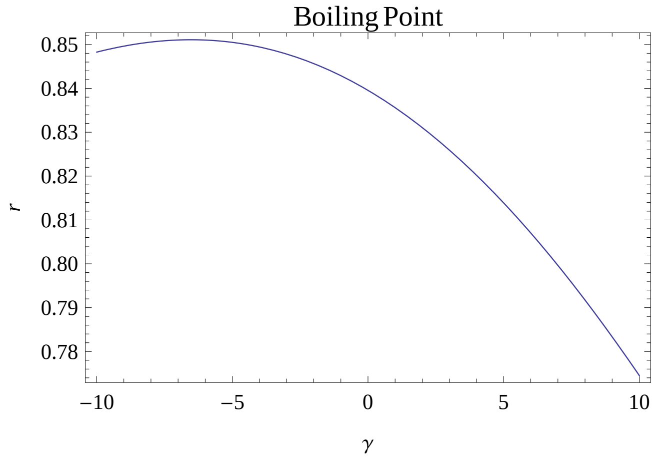

Figure 1. The positive values of the correlation r (between the boiling point of the considered compounds and ABS_γ) when $\gamma \in [-10, 10]$.

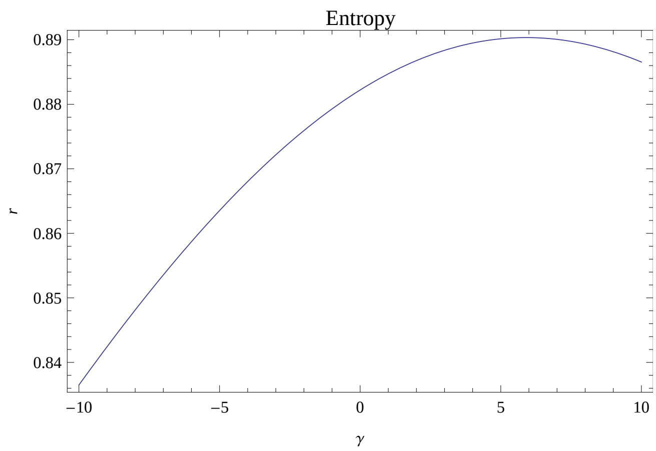

Figure 2. The positive values of the correlation r (between the entropy of the considered compounds and ABS_γ) when $\gamma \in [-10, 10]$.

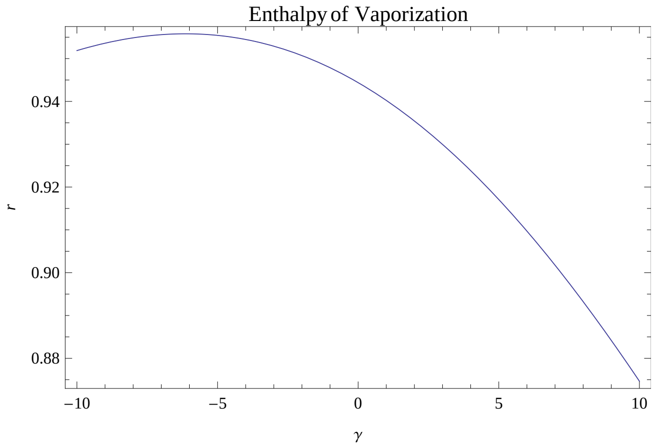

Figure 3. The positive values of the correlation r (between the enthalpy of vaporization of the considered compounds and ABS_γ) when $\gamma \in [-10, 10]$.

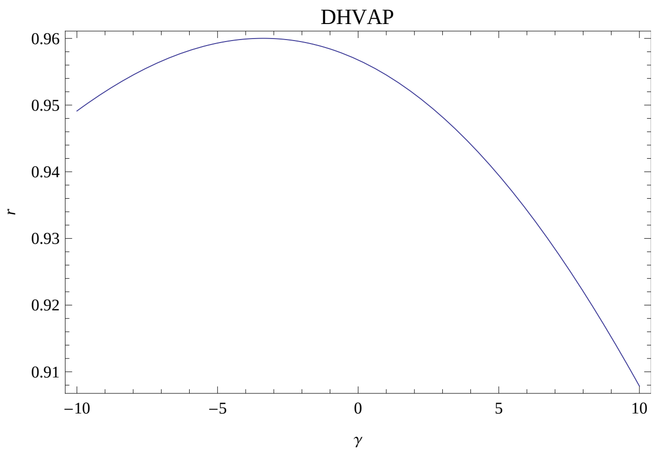

Figure 4. The positive values of the correlation r (between the standard enthalpy of vaporization (DHVAP) of the considered compounds and ABS_γ) when $\gamma \in [-10, 10]$.

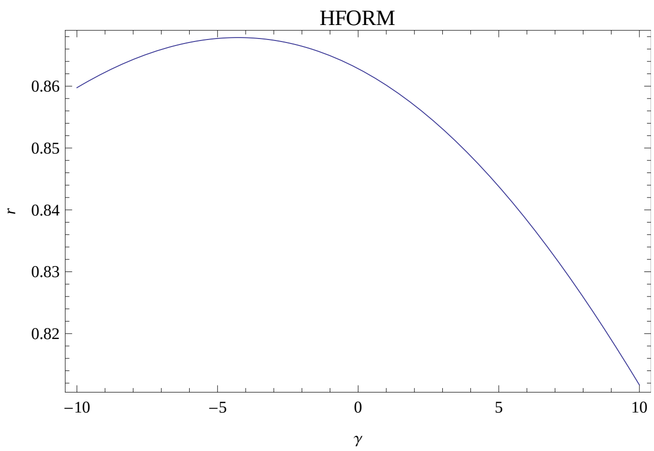

Figure 5. The positive values of the correlation r (between the enthalpy of formation (HFORM) of the considered compounds and ABS_γ) when $\gamma \in [-10, 10]$.

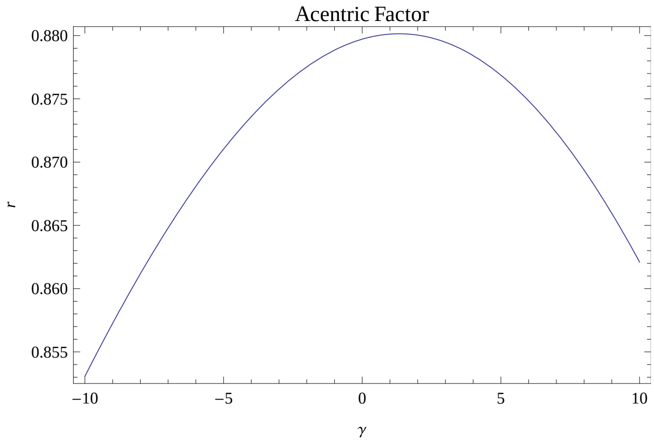

Figure 6. The positive values of the correlation r (between the acentric factor of the considered compounds and ABS_γ) when $\gamma \in [-10, 10]$.

Table 1. The maximum positive values of the correlation r, between the selected properties of octane isomers and ABS_γ, when $\gamma \in [-10, 10]$.

	r	γ
Boiling point	0.8511	-6.5275
Enthalpy of vaporization	0.9558	-6.1399
Standard enthalpy of vaporization	0.9600	-3.3760
Entropy	0.8903	5.9019
Acentric factor	0.8801	1.3381
Enthalpy of formation	0.8679	-4.2677

Table 2. The maximum positive values of the correlation r, between the selected properties of octane isomers and ABS_γ, when $\gamma \in [-3, 3]$.

	r	γ
Boiling point	0.8478	-3.0000
Enthalpy of vaporization	0.9529	-3.0000
Standard enthalpy of vaporization	0.9600	-3.0000
Entropy	0.8884	3.0000
Acentric factor	0.8801	1.3381
Enthalpy of formation	0.8674	-3.0000

In Tables 1 and 2, corresponding to every listed property, we observe that there is only a slight difference between the two values of r. (For example, in the case of boiling point, the mentioned difference is 0.0033.) However, there is a considerable difference between the corresponding two values of γ. In view of these observations, we conclude that the approximated values of γ concerning any promising results belong to the set $\{-3, 1, 3\}$. These findings suggest that the following three particular versions of ABS_γ deserve to be examined further:

(i) The topological index ABS_1 is useful in predicting the acentric factor of octane isomers. It seems to be interesting to note that

$$ABS_1(G) = \sum_{st\in E(G)} \left(1 - \frac{2}{d_s + d_t}\right) = |E(G)| - H(G),$$

where $H(G)$ is the harmonic index, first appeared in [8].

(ii) The topological index ABS_{-3} is useful in predicting the enthalpy of vaporization, boiling point, enthalpy of formation and standard enthalpy of vaporization of octane isomers.

(iii) The topological index ABS_3 is useful in predicting the entropy of octane isomers.

3. On the index ABS_γ and addition of an edge in a graph

For a graph G and $st \notin E(G)$, the graph generated from G by inserting the edge st is represented by $G + st$. In this section, the difference $ABS_\gamma(G + st) - ABS_\gamma(G)$ is investigated. We start with the following known result.

Corollary 3.1. *[1] For a graph G, if $st \notin E(G)$ such that $\max\{d_s(G), d_t(G)\} \geq 1$, then,*

$$ABS_\gamma(G + st) > ABS_\gamma(G) \quad \text{for } \gamma \geq 0.$$

Proposition 3.1. *For a graph G, if $st \notin E(G)$ such that $d_s(G) = 1$ and $d_t(G) = 0$, then,*

$$ABS_\gamma(G + st) > ABS_\gamma(G) \quad \text{for every } \gamma.$$

Proof. If $\gamma \geq 0$, then the required conclusion follows from Corollary 3.1. In the remaining proof, suppose that $\gamma < 0$. By the definition of ABS_γ, G contains no component isomorphic to K_2 and it holds that

$$ABS_\gamma(G + st) - ABS_\gamma(G) = \left(\frac{d_{s'}(G)}{d_{s'}(G) + 2}\right)^\gamma - \left(\frac{d_{s'}(G) - 1}{d_{s'}(G) + 1}\right)^\gamma + \left(\frac{1}{3}\right)^\gamma, \tag{3.1}$$

where s' is the unique vertex adjacent with s in G. Since the degree of s is 1 in G (and $\gamma < 0$), by the definition of ABS_γ we must have $d_{s'}(G) > 1$ (for otherwise G contains a component isomorphic to K_2). Note that the function ϕ_γ, with the following definition, is strictly increasing for $\alpha > 1$:

$$\phi_\gamma(\alpha) = \left(\frac{\alpha}{\alpha + 2}\right)^\gamma - \left(\frac{\alpha - 1}{\alpha + 1}\right)^\gamma,$$

because its derivative function ϕ'_γ is

$$\phi'_\gamma(\alpha) = 2\gamma\Big(f_\gamma(\alpha + 1) - f_\gamma(\alpha)\Big),$$

where

$$f_\gamma(\alpha) = \frac{(\alpha - 1)^{\gamma-1}}{(\alpha + 1)^{\gamma+1}} \text{ and } f'_\gamma(\alpha) = \frac{2(\gamma - \alpha)(\alpha - 1)^{\gamma-2}}{(\alpha + 1)^{\gamma+2}} < 0, \quad \text{for } \gamma < 0 \text{ and } \alpha > 1.$$

Consequently,

$$\left(\frac{d_{s'}}{d_{s'}+2}\right)^{\gamma}-\left(\frac{d_{s'}-1}{d_{s'}+1}\right)^{\gamma}+\left(\frac{1}{3}\right)^{\gamma}=\phi_{\gamma}(d_{s'})+\left(\frac{1}{3}\right)^{\gamma}\geq\phi_{\gamma}(2)+\left(\frac{1}{3}\right)^{\gamma}>0,$$

which together with Eq (3.1) give $ABS_{\gamma}(G+st)-ABS_{\gamma}(G)>0$.

For a graph G and $w\in V(G)$, let $N_G(w)=\{x\in V(G):xw\in E(G)\}$.

Proposition 3.2. *For a graph G, if $st\notin E(G)$ such that $d_s(G)=d_t(G)=1$, then,*

$$ABS_{\gamma}(G+st)>ABS_{\gamma}(G)\quad \textit{for}\ \gamma>-1.$$

Proof. If $\gamma\geq 0$, then the required conclusion follows from Corollary 3.1. In the following, we assume that $-1<\gamma<0$. Take $N_G(s)=\{s'\}$ and $N_G(t)=\{t'\}$. Since $d_s(G)=1=d_t(G)$ and $-1<\gamma<0$, by the definition of ABS_{γ}, we must have $\min\{d_{s'}(G),d_{t'}(G)\}>1$ (for otherwise G contains a component isomorphic to K_2). Note that the function ϕ_{γ}, with the following definition, is strictly increasing for $\alpha>1$ and $\gamma<0$ (see the proof of Proposition 3.1):

$$\phi_{\gamma}(\alpha)=\left(\frac{\alpha}{\alpha+2}\right)^{\gamma}-\left(\frac{\alpha-1}{\alpha+1}\right)^{\gamma}.$$

Thus, for $-1<\gamma<0$, we have

$$\begin{aligned}
&ABS_{\gamma}(G+st)-ABS_{\gamma}(G)\\
=&\left(\frac{d_{s'}(G)}{d_{s'}(G)+2}\right)^{\gamma}-\left(\frac{d_{s'}(G)-1}{d_{s'}(G)+1}\right)^{\gamma}+\left(\frac{d_{t'}(G)}{d_{t'}(G)+2}\right)^{\gamma}-\left(\frac{d_{t'}(G)-1}{d_{t'}(G)+1}\right)^{\gamma}+\left(\frac{1}{2}\right)^{\gamma}\\
=&\phi_{\gamma}(d_{s'})+\phi_{\gamma}(d_{t'})+\left(\frac{1}{2}\right)^{\gamma}\\
\geq&2\phi_{\gamma}(2)+\left(\frac{1}{2}\right)^{\gamma}>0.
\end{aligned}$$

Although the next result's proof is similar to the proof of Proposition 3.2, we include it here for completeness.

Proposition 3.3. *For a graph G, if $st\notin E(G)$ such that both the vertices s,t have degree 1 (in G) and that one of their unique neighbors has a degree greater than 3 (in G) and the other unique neighbor has a degree greater than 2 (in G), then,*

$$ABS_{\gamma}(G+st)>ABS_{\gamma}(G)\quad \textit{for every}\ \gamma.$$

Proof. If $\gamma\geq 0$, then the required conclusion follows from Corollary 3.1. In the following, we assume $\gamma<0$. Take $N_G(s)=\{s'\}$ and $N_G(t)=\{t'\}$. By the given constraints, $\min\{d_{s'}(G),d_{t'}(G)\}>2$ and $\max\{d_{s'}(G),d_{t'}(G)\}>3$. Note that the function ϕ_{γ}, with the following definition, is strictly increasing for $\alpha>1$ and $\gamma<0$ (see the proof of Proposition 3.1):

$$\phi_{\gamma}(\alpha)=\left(\frac{\alpha}{\alpha+2}\right)^{\gamma}-\left(\frac{\alpha-1}{\alpha+1}\right)^{\gamma}.$$

Thus, for $\gamma < 0$, we have

$$\begin{aligned}
&ABS_\gamma(G+st) - ABS_\gamma(G)\\
=&\left(\frac{d_{s'}(G)}{d_{s'}(G)+2}\right)^\gamma - \left(\frac{d_{s'}(G)-1}{d_{s'}(G)+1}\right)^\gamma + \left(\frac{d_{t'}(G)}{d_{t'}(G)+2}\right)^\gamma - \left(\frac{d_{t'}(G)-1}{d_{t'}(G)+1}\right)^\gamma + \left(\frac{1}{2}\right)^\gamma\\
=&\phi_\gamma(d_{s'}) + \phi_\gamma(d_{t'}) + \left(\frac{1}{2}\right)^\gamma\\
\geq&\phi_\gamma(3) + \phi_\gamma(4) + \left(\frac{1}{2}\right)^\gamma > 0.
\end{aligned}$$

4. Extremal results

In the current section, we characterize the graphs possessing the maximum value of ABS_γ, with $\gamma > 0$, in the set of all connected graphs of a fixed order and a fixed (i) vertex connectivity not greater than a given number or (ii) matching number. The following lemma is very crucial in proving the first main result of this section.

Lemma 4.1. *Define the functions Φ_1 and Φ_2 as*

$$\Phi_1(x) = \left(\frac{t+x-2}{t+x-1}\right)^\gamma \frac{x(x-1)}{2}$$

and

$$\Phi_2(x) = \left(\frac{x+n+t-4}{x+n+t-2}\right)^\gamma t\,x$$

with the constraint $1 \leq x \leq \frac{n-t}{2}$, where γ is a fixed positive real number greater than zero, while t and n are fixed positive integers. Define $\Phi(x) = \Phi_1(x)+\Phi_2(x)$. If either of the following two conditions holds:

(i) $t \geq 2$;

(ii) $2 \leq x \leq \dfrac{n-t}{2}$ *and* $t = 1$,

then, the inequality

$$\Phi(n-t-x) + \Phi(x) \leq \Phi(n-t-1) + \Phi(1)$$

holds with equality if and only if $x = 1$.

Proof. First, we assume that $t \geq 2$. The second-derivative function Φ_1'' of Φ_1 is given as

$$\Phi_1''(x) = \frac{\Psi_1(x)}{2(t+x-2)^2(t+x-1)^2}\left(\frac{t+x-2}{t+x-1}\right)^\gamma,$$

where

$$\begin{aligned}
\Psi_1(x) = \gamma\Big(2t^2(2x-1) + 2t\big(x(3x-7)+3\big) + (x-1)\big(x(2x-7)+4\big)\Big)&\\
+ 2(t+x-2)^2(t+x-1)^2 + \gamma^2(x-1)x.&
\end{aligned}$$

In the expression of Ψ_1, note that the coefficient of γ attains its minimum value at $t = 2$ and hence is positive (because $t \geq 2$ and $x \geq 1$). Thus, $\Psi_1(x) > 0$ (as $\gamma > 0$), and therefore $\Phi_1''(x) > 0$. Additionally, the second-derivative function Φ_2'' of Φ_2 is given as

$$\Phi_2''(x) = \frac{4\gamma t \cdot \Psi_2(x)}{(n+t+x-4)^2(n+t+x-2)^2}\left(\frac{n+t+x-4}{n+t+x-2}\right)^{\gamma},$$

where

$$\Psi_2(x) = n^2 + n(2t + x - 6) + t(t + x - 6) + \gamma x - 3x + 8.$$

Here, $\Psi_2'(x) = n + t + \gamma - 3 > 0$ because $n \geq 4$, $t \geq 2$ and $\gamma > 0$. Since $x \geq 1$, we have

$$\Psi_2(x) \geq \Psi_2(1) = (n-4)(n-1) + t(2n + t - 5) + \gamma + 1 > 0.$$

Therefore, it holds that $\Phi_2''(x) > 0$. Because $\Phi(x) = \Phi_1(x) + \Phi_2(x)$, we conclude that the first-derivative function Φ' of Φ is strictly increasing. Since $x \leq n - t - x$, we have

$$\frac{d}{dx}(\Phi(x) + \Phi(n-t-x)) = \Phi'(x) - \Phi'(n-t-x) \leq 0,$$

where the equality

$$\frac{d}{dx}(\Phi(x) + \Phi(n-t-x)) = 0$$

holds if and only if $x = n - t - x$. Consequently, we deduce that the expression $\Phi(x) + \Phi(n - t - x)$ attains its maximum possible value only at $x = 1$.

The desired inequality when $2 \leq x \leq \frac{n-t}{2}$ and $t = 1$ remains to be proved. In what follows, it is assumed that $2 \leq x \leq \frac{n-t}{2}$ and $t = 1$. The second-derivative function Φ_1'' of Φ_1 is given as

$$\Phi_1''(x) = \frac{(x-1)^{\gamma-1}x^{-\gamma-1}}{2}\left(2x(x-1) + \gamma(2x-1) + \gamma^2\right),$$

which is certainly positive (because $\gamma > 0$ and $x \geq 2$). Additionally, the second-derivative function Φ_2'' of Φ_2 is given as

$$\Phi_2''(x) = 4\gamma\left(\frac{n+x-3}{n+x-1}\right)^{\gamma}\frac{n(n-4) + x(n-2) + \gamma x + 3}{(n+x-3)^2(n+x-1)^2},$$

which is positive too because $n \geq 5$, $x \geq 2$ and $\gamma > 0$. Thus, in the case under consideration, the expression $\Phi(x) + \Phi(n - 1 - x)$ attains its maximum possible value only at $x = 2$. Thus, in order to complete the proof, it is enough to show that

$$\Phi(2) + \Phi(n-3) - \Phi(1) - \Phi(n-2) < 0.$$

Take $\Theta(n, \gamma) = \Phi(2) + \Phi(n - 3) - \Phi(1) - \Phi(n - 2)$. Then, we have

$$\begin{aligned}\Theta(n,\gamma) = &\left[\left(\frac{1}{2}\right)^{\gamma} - \left(\frac{n-2}{n}\right)^{\gamma}\right] + \frac{(n-4)(n-3)}{2}\left[\left(\frac{n-4}{n-3}\right)^{\gamma} - \left(\frac{n-3}{n-2}\right)^{\gamma}\right]\\ &+ \left[2\left(\frac{n-1}{n+1}\right)^{\gamma} - (n-2)\left(\frac{2n-5}{2n-3}\right)^{\gamma}\right]. \end{aligned} \tag{4.1}$$

Since

$$\left(\frac{n-1}{n+1}\right)^{\gamma} < \left(\frac{2n-5}{2n-3}\right)^{\gamma} \quad \text{for } n \geq 5 \text{ and } \gamma > 0,$$

it holds that

$$2\left(\frac{n-1}{n+1}\right)^{\gamma} < (n-2)\left(\frac{n-1}{n+1}\right)^{\gamma} < (n-2)\left(\frac{2n-5}{2n-3}\right)^{\gamma} \quad \text{for } n \geq 5 \text{ and } \gamma > 0.$$

Additionally, for $n \geq 5$ and $\gamma > 0$, we have

$$\left(\frac{1}{2}\right)^{\gamma} < \left(\frac{n-2}{n}\right)^{\gamma}$$

and

$$\left(\frac{n-4}{n-3}\right)^{\gamma} < \left(\frac{n-3}{n-2}\right)^{\gamma}.$$

Therefore, Eq (4.1) yields $\Theta(n,\gamma) < 0$, as desired.

Theorem 4.1. *In the set of all n-order connected graphs having the vertex connectivity at most t (being a positive integer satisfying $1 \leq t \leq n-2$), the graph $K_n^{(t)}$ uniquely possesses the largest value of ABS_γ for $\gamma > 0$, where $n \geq 5$ and $K_n^{(t)}$ is the graph formed by joining a new vertex (through edges) to exactly t vertices of the complete graph K_{n-1}. The mentioned maximum value is as follows:*

$$ABS_\gamma\left(K_n^{(t)}\right) = \left(\frac{n-2}{n-1}\right)^{\gamma} \frac{t(t-1)}{2} + t\left(\frac{t+n-3}{t+n-1}\right)^{\gamma} + \frac{(n-t-2)(n-t-1)}{2}\left(\frac{n-3}{n-2}\right)^{\gamma} + (n-t-1)t\left(\frac{2n-5}{2n-3}\right)^{\gamma}.$$

Proof. First, we consider a positive integer s less than t. Observe that $K_n^{(t)}$ can be formed by adding some edge(s) in the graph $K_n^{(s)}$. Thus, by Corollary 3.1, the inequality $ABS_\gamma\left(K_n^{(s)}\right) < ABS_\gamma\left(K_n^{(t)}\right)$ holds for $\gamma > 0$. Consequently, it is adequate to prove the theorem only for the n-order connected graphs having the vertex connectivity t.

Let G^* be a graph possessing the largest value of ABS_γ in the set of all n-order connected graphs having the vertex connectivity t for $\gamma > 0$, where $n \geq 5$ and $1 \leq t \leq n-2$. Since the vertex connectivity of G^* is t, there exists a subset A of the vertex set of G^* such that $|A| = t$ and $G^* - A$ consists of at least two components, where $G^* - A$ is the graph formed from G^* by removing all the vertices (and their incident edges) of A. If the graph $G^* - A$ has more than two components, then adding an edge connecting the vertices lying in two different components of $G^* - A$ increases the value of $ABS_\gamma(G^*)$ (by Corollary 3.1); however, the vertex connectivity of G^* remains the same, which is antithetical to the maximality of $ABS_\gamma(G^*)$. Thereby, the graph $G^* - A$ must have only two components; we name them as C_1 and C_2. Additionally, by Corollary 3.1, the graphs C_1, C_2 and $G^*[A]$ are complete, and every vertex of both the components C_1, C_2, is adjacent to every vertex of the set A in G^*, where $G^*[A]$ is the induced subgraph of G formed on the vertices of A. For $i \in \{1, 2\}$, let c_i be the order of C_i and suppose that $c_1 \leq c_2$. Then, $t + c_1 + c_2 = n$ and $c_1 \leq \frac{n-t}{2}$. Note that the degree of every vertex belonging to C_i is

$c_i - 1 + t$ in G^*, where $i = 1, 2$. Moreover, the degree of every vertex belonging to A is $n-1$ in G^*. By utilizing the formula of ABS_γ, we obtain the following:

$$ABS_\gamma(G^*) = \left(\frac{t+c_1-2}{t+c_1-1}\right)^\gamma \frac{c_1(c_1-1)}{2} + \left(\frac{n+t+c_1-4}{n+t+c_1-2}\right)^\gamma c_1 t + \left(\frac{t+c_2-2}{t+c_2-1}\right)^\gamma \frac{c_2(c_2-1)}{2}$$
$$+ \left(\frac{n+t+c_2-4}{n+t+c_2-2}\right)^\gamma c_2 t + \left(\frac{n-2}{n-1}\right)^\gamma \frac{t(t-1)}{2}.$$

By making use of the definition of the function Φ defined in Lemma 4.1, we obtain the following:

$$ABS_\gamma(G^*) = \Phi(c_1) + \Phi(c_2) + \left(\frac{n-2}{n-1}\right)^\gamma \frac{t(t-1)}{2}.$$

Utilizing the fact that $c_2 = n - c_1 - t$, we arrive at the following:

$$ABS_\gamma(G^*) = \Phi(c_1) + \Phi(n-t-c_1) + \left(\frac{n-2}{n-1}\right)^\gamma \frac{t(t-1)}{2}.$$

By making use of Lemma 4.1 and the definition of G^*, we conclude that

$$\begin{aligned} ABS_\gamma(G^*) &= \Phi(c_1) + \Phi(n-t-c_1) + \left(\frac{n-2}{n-1}\right)^\gamma \frac{t(t-1)}{2} \\ &= \Phi(1) + \Phi(n-t-1) + \left(\frac{n-2}{n-1}\right)^\gamma \frac{t(t-1)}{2}, \end{aligned}$$

which implies that $c_1 = 1$ and thereby the graph G^* is isomorphic to $K_n^{(t)}$. Hence,

$$ABS_\gamma\left(K_n^{(t)}\right) = \Phi(1) + \Phi(n-t-1) + \left(\frac{n-2}{n-1}\right)^\gamma \frac{t(t-1)}{2}.$$

or

$$ABS_\gamma\left(K_n^{(t)}\right) = \left(\frac{n-2}{n-1}\right)^\gamma \frac{t(t-1)}{2} + t\left(\frac{t+n-3}{t+n-1}\right)^\gamma + \frac{(n-t-2)(n-t-1)}{2}\left(\frac{n-3}{n-2}\right)^\gamma$$
$$+ (n-t-1)t\left(\frac{2n-5}{2n-3}\right)^\gamma.$$

A component C of a graph is said to be an odd component if the order of C is odd. Let $\mathcal{CG}_{n,\beta}$ be the set of all connected n-order graphs having a matching number β, where $1 \le \beta \le \lfloor n/2 \rfloor$ (this condition is imposed because the matching number of any n-order connected graph cannot be greater than $\lfloor n/2 \rfloor$). Note that the n-order complete graph K_n has the matching number $\lfloor n/2 \rfloor$. Thus, by Corollary 3.1, K_n uniquely possesses the largest value of ABS_γ over $\mathcal{CG}_{n,\lfloor n/2 \rfloor}$ for $\gamma > 0$. Thereby, in the next result, we consider the case when $1 \le \beta \le \lfloor n/2 \rfloor - 1$.

Theorem 4.2. *In the set $\mathcal{CG}_{n,\beta}$, the graph $\overline{K}_{n-\beta} + K_\beta$ uniquely possesses the largest value of ABS_γ for $\gamma > 0$, where $\overline{K}_{n-\beta}$ denotes the complement of the complete graph $K_{n-\beta}$, "+" denotes the graph-operation join, $1 \le \beta \le \lfloor n/2 \rfloor - 1$ and $n \ge 5$. Additionally, the mentioned maximum value is as follows:*

$$ABS_\gamma\left(\overline{K}_{n-\beta} + K_\beta\right) = \left(\frac{n-2}{n-1}\right)^\beta \frac{\beta(\beta-1)}{2} + \left(\frac{\beta+n-3}{\beta+n-1}\right)^\alpha (n-\beta)\beta.$$

Proof. Let G^* be a graph possessing the maximum value of ABS_γ in the set $\mathcal{CG}_{n,\beta}$ for $\gamma > 0$, provided that $1 \le \beta \le \lfloor n/2 \rfloor - 1$ and $n \ge 5$. The Tutte-Berge formula (see [14]) confirms that the vertex set $V(G^*)$ has a subset W such that

$$n - 2\beta = o(G^* - W) - |W|, \tag{4.2}$$

where $o(G^* - W)$ is the number of odd components of the graph $G^* - W$ (which is the graph formed by dropping all the vertices (and the edges incident with them) of W from G^*). Note that

$$n \ge o(G^* - W) + |W|,$$

which together with (4.2) imply that $\beta \ge |W|$.

If $|W| = 0$, then from Eq (4.2), we deduce that either $n = 2\beta$ or $n = 2\beta + 1$ because G^* is connected. Whether $n = 2\beta$ or $n = 2\beta + 1$, one has $\lfloor n/2 \rfloor = \beta$, which is impossible under the given constraints. Thus, $\beta \ge |W| \ge 1$, and from Eq (4.2), we get $o(G^* - W) \ge 3$ because $\beta \le \lfloor n/2 \rfloor - 1$.

Let $G_1^*, \ldots, G_q^*$ be odd components of the graph $G^* - W$, where $q = o(G^* - W) \ge 3$. For $i = 1, \ldots, q$, suppose that G_i^* has r_i vertices and assume that $r_q \ge r_{q-1} \ge \cdots \ge r_1$. Now, we show that the graph $G^* - W$ does not have any even component. On the contrary, suppose that G_{q+1}^* is an even component of the graph $G^* - W$. Construct a new graph G^{**} from G^* by adding an edge $w_1 w_{q+1}$ such that $w_{q+1} \in V(G_{q+1}^*)$ and $w_1 \in V(G_1^*)$. Then, certainly we have $\beta(G^{**}) \ge \beta(G^*)$. Moreover, by the Tutte-Berge formula, we have the following:

$$o(G^{**} - W) - |W| \le n - 2\beta(G^{**}). \tag{4.3}$$

Note that $o(G^{**} - W) = o(G^* - W)$, which together with Eq (4.2) implies that

$$o(G^{**} - W) - |W| = n - 2\beta(G^*);$$

this last equation and (4.3) yield $\beta(G^*) \ge \beta(G^{**})$. Thus, $\beta(G^{**}) = \beta(G^*)$. However, by Corollary 3.1, it holds that $ABS_\gamma(G^*) < ABS_\gamma(G^{**})$ for $\gamma > 0$, which is antithetical to the maximality of $ABS_\gamma(G^*)$. Therefore, the graph $G^* - W$ does not possess any even component.

By Corollary 3.1, each of the graphs G_i^* (for $i = 1, \ldots, q$) and $G^*[W]$ is complete, and every vertex of W is adjacent to every vertex of all the graphs $G_1^*, \ldots, G_q^*$. Therefore, $G^* = \left(K_{r_1} \cup \cdots \cup K_{r_q}\right) + K_p$, where $1 \le p = |W| \le \beta$; $o(G^* - W) = q \ge 3$; $\sum_{i=1}^{q} r_i + p = n$; $n - 2\beta = q - p$ and each of the numbers $r_1, r_2, \ldots, r_q$ is odd, with $r_q \ge r_{q-1} \ge \cdots \ge r_1$.

Case 1. When $r_q = 1$.

In this case, $r_q = r_{q-1} = \cdots = r_1 = 1$ and $p = \beta$. Since $n - 2\beta = q - p$, we have $G^* = \overline{K}_{n-\beta} + K_\beta$, as desired.

Case 2. When $r_q \ge 3$ and $r_{q-1} = 1$.

In this case, $r_{q-1} = \cdots = r_1 = 1$. From the equations $\sum_{i=1}^{q} r_i + p = n$ and $n - 2\beta = q - p$, we get $r_q = 1 - 2p + 2\beta$ (which implies that $\beta > p$ because $r_q \ge 3$). Thus,

$$G^* = (\overline{K}_{q-1} \cup K_{r_q}) + K_p = (\overline{K}_{n+p-2\beta-1} \cup K_{1-2p+2\beta}) + K_p. \tag{4.4}$$

Observe that $(\overline{K}_{n+p-2\beta-1} \cup K_{1-2p+2\beta}) + K_p$ is a spanning subgraph of the graph $\overline{K}_{n-\beta} + K_\beta$ and thus by making use of Corollary 3.1, we deduce that

$$ABS_\gamma(G^*) = ABS_\gamma\left((\overline{K}_{n+p-2\beta-1} \cup K_{1-2p+2\beta}) + K_p\right) < ABS_\gamma\left(\overline{K}_{n-\beta} + K_\beta\right)$$

for $\gamma > 0$. This is antithetical to the maximality of G^*. Therefore, this case is not possible.

Case 3. When $r_{q-1} \geq 3$.

In this case, $r_q \geq 3$ as $r_q \geq r_{q-1}$. Take

$$\Theta = ABS_\gamma\left(\left(K_{r_1} \cup \cdots \cup K_{r_{q-2}} \cup K_1 \cup K_{r_q+r_{q-1}-1}\right) + K_p\right) - ABS_\gamma(G^*). \tag{4.5}$$

After elementary computations, we obtain

$$\begin{aligned}
\Theta =&\left(\frac{p+n-3}{p+n-1}\right)^\gamma p + \left(\frac{p+r_q+r_{q-1}-3}{p+r_q+r_{q-1}-2}\right)^\gamma \frac{(r_q+r_{q-1}-1)\left(r_q+r_{q-1}-2\right)}{2}\\
&+\left(\frac{p+r_q+r_{q-1}+n-5}{p+r_q+r_{q-1}+n-3}\right)^\gamma (r_q+r_{q-1}-1)p\\
&-\left(\frac{p+r_{q-1}-2}{p+r_{q-1}-1}\right)^\gamma \frac{r_{q-1}\left(r_{q-1}-1\right)}{2} + \left(\frac{p+r_{q-1}+n-4}{p+r_{q-1}+n-2}\right)^\gamma r_{q-1}p\\
&-\left(\frac{p+r_q-2}{p+r_q-1}\right)^\gamma \frac{r_q\left(r_q-1\right)}{2} + \left(\frac{p+r_q+n-4}{p+r_q+n-2}\right)^\gamma r_q p\\
=&\Phi(1) + \Phi(r_q+r_{q-1}-1) - \Phi(r_{q-1}) - \Phi(r_q),
\end{aligned}$$

where the definition of the function Φ is given in Lemma 4.1. Set $r_q + r_{q-1} + \beta = n'$. Then $r_{q-1} \leq \frac{n'-\beta}{2}$ because $r_{q-1} \leq r_q$. Thus,

$$\Theta = \Phi(1) + \Phi(n'-\beta-1) - \Phi(r_{q-1}) - \Phi(n'-\beta-r_{q-1}),$$

and by Lemma 4.1, the right-handed expression of this equation is greater than 0. Therefore, Eq (4.5) yields a contradiction to the maximality of $ABS_\gamma(G^*)$. Consequently, this case is also impossible.

5. Conclusions

In this paper, the chemical usefulness and several mathematical aspects of the index ABS_γ have been considered and studied. For $-10 \leq \gamma \leq 10$, the significance of ABS_γ is examined on the data set of octane isomers for predicting six selected physicochemical properties of the mentioned compounds; promising results are obtained when the approximated value of γ belongs to the set $\{-3, 1, 3\}$. (The selected six properties are the following: enthalpy of vaporization, boiling point, acentric factor, enthalpy of formation, entropy, and standard enthalpy of vaporization.) The value $\gamma = 1$ corresponds to the index that can be written in the form of an existing index, namely the harmonic index. The findings of Section 2 indicate that the topological indices ABS_1 and ABS_3 are useful in predicting the acentric factor and the entropy of octane isomers, respectively; the index ABS_{-3} can be utilized to predict the remaining four selected properties (enthalpy of vaporization, boiling point, enthalpy of formation, and standard enthalpy of vaporization) of octane isomers. The effect of the addition of an edge between two non-adjacent vertices of a graph under ABS_γ has also been investigated. Moreover, the graphs possessing the maximum value of ABS_γ, with $\gamma > 0$, are characterized from the set of all connected graphs of a fixed order and a fixed (i) vertex connectivity not greater than a given number or (ii) matching number. From the above-mentioned set of three values of γ, the choices $\gamma = -3, 3$, yield two new indices with promising chemical usefulness. Thus, these two indices, namely ABS_{-3} and ABS_3, deserve to be examined further.

Use of AI tools declaration

The authors declare they have not used Artificial Intelligence (AI) tools in the creation of this article.

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Conflict of interest

The authors declare that they have no conflicts of interest.

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