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Research article

The spectral radius and energy for atom-bond sum-connectivity matrix

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Abstract: This paper investigates the spectral radius and energy of the atom-bond sum-connectivity (ABS) matrix. Through rigorous mathematical analysis, we establish bounds for the ABS spectral radius across several graph classes and investigate its properties. The ABS energy is defined, and its calculation methods and properties are studied. Furthermore, by analyzing the correlation between the ABS spectral radius and the physicochemical properties of octane isomers, it is revealed that the ABS spectral radius performs well in predicting molecular properties, indicating its potential application value in chemical structure-property modeling.

Keywords: ABS index; ABS spectral radius; ABS energy; ABS matrix; correlation analysis
Mathematics Subject Classification: 05C15, 05C22, 05C31

1. Introduction

Consider a graph $G = (V(G), E(G))$, where the vertex set is by $V(G) = \{v_1, v_2, \ldots, v_n\}$, and the edge set is $E(G)$. We use the notation $i \sim j$ to signify that $v_iv_j \in E(G)$. For vertex $v_i \in V(G)$, its degree d_i is defined as the number of edges that are incident to v_i. The maximum degree of the graph G is denoted by Δ, such that $\Delta = \max\{d_i\}$, and the minimum degree is denoted by δ, with $\delta = \min\{d_i\}$. The cycle, star, and path, each having n vertices, are represented by C_n, S_n, and P_n, in that order. The bipartite semiregular graph is a special type of bipartite graph whose vertex set can be partitioned into two disjoint subsets such that all vertices within the same subset have the same degree, but the degrees of the two subsets may differ.

Within mathematical chemistry, the construction of mathematical models to elucidate the relationships between molecular structures and the physicochemical properties of compounds represents a prevalent approach for exploring quantitative structure-activity relationships (QSAR) and quantitative structure-property relationships (QSPR). Consequently, numerous molecular graph-based structure descriptors have been proposed. In [1], the authors reviewed the use of quantum-chemical descriptors in QSAR/QSPR studies, highlighting their critical role in establishing correlations with

biological activity, chemical reactivity, partition coefficients, and other physicochemical properties. [2] covered statistical modeling methods for molecular descriptors in QSAR/QSPR, including statistical, information-theoretic, and data analysis techniques for building data-driven predictive models of molecular properties and structure. Topological indices (TI) are numerical descriptors associated with the molecular architecture of chemical compounds. Leveraging mathematical formalisms, these indices offer a quantitative representation of molecular structural characteristics. They enable a comprehensive understanding of the diverse physicochemical properties and biological activities of molecules, facilitating a deeper exploration of their behavior and interactions in various contexts. For example, [3] used graph theory to analyze how the molecular structure of alternant hydrocarbons determines their total π-electron energy. Thus, in mathematical chemistry, one can represent a topological index in matrix form (e.g., the weighted adjacency matrix [4]) and utilize its eigenvalues to predict the physicochemical properties of molecules.

In 1975, Randić [5] proposed a method for characterizing the branching of molecules, which laid the foundation for subsequent research. Since then, the Randić index and its related theories have been widely studied and developed. Gutman and Furtula's summary and review of theoretical advances in the Randić index [6] further advanced the field. The Randić index is:

$$R(G) = \sum_{i\sim j} \frac{1}{\sqrt{d_i d_j}}.$$

In addition to the Randić index, other topological indices have also attracted widespread attention. Proposed by Estrada et al. in 1998 [7], the atom-bond connectivity (ABC) index is intended to predict the formation of enthalpy of alkanes.

$$ABC(G) = \sum_{i\sim j} \sqrt{\frac{d_i + d_j - 2}{d_i d_j}}.$$

The ABC index provides a new perspective on the relationship between molecular structure and energy properties by considering the interactions between atoms and bonds. Subsequently, Zhou and Trinajstić [8] introduced a new index, called the sum-connectivity (SC) index, which further enriched the research of the topological index.

$$SC(G) = \sum_{i\sim j} \frac{1}{\sqrt{d_1 + d_j}}.$$

The atom-bond sum-connectivity (ABS) index was introduced in [9]. [10] investigated the relationship between the general sum-connectivity index and the connectivity of a graph, establishing new bounds for the sum-connectivity index.

$$ABS(G) = \sum_{i\sim j} \sqrt{\frac{d_i + d_j - 2}{d_i + d_j}}.$$

To facilitate further analysis, the ABS-matrix is denoted by $S = S(G) = \left[a_{ij}\right]_{n\times n}$, where

$$a_{ij} = \begin{cases} \sqrt{\frac{d_i+d_j-2}{d_i+d_j}}, & v_i v_j \in E(G); \\ 0, & otherwise. \end{cases}$$

We define the eigenvalues of $S(G)$ as $\rho_1(S(G)) \geq \rho_2(S(G)) \geq \cdots \geq \rho_n(S(G))$, and denote ABS eigenvalues of G. Among them, the largest eigenvalue, referred to as the ABS spectral radius, is denoted by $\rho(S(G))$.

In [11], the ABC index was combined with matrix theory to reveal the structural features of graphs through spectral analysis, thus providing insight into the potential relationship between graph-theoretic properties and molecular structure. [12] discussed corrections to previously reported bounds on the ABC index of graphs, addressing errors in earlier publications. [13] examined the ABC index of trees with a fixed number of leaves. [14] reviewed the extremal results and bounds of the ABC index in graph theory, as well as its applications in chemistry. [15] examined the ABC index in chemical trees, focusing on its minimum and maximum values and their significance. [16] discussed the extremality of the ABC spectral radius of a tree, proving that for any tree of order $n \geq 3$, the ABC spectral radius satisfies a specific inequality if and only if the tree is isomorphic to a particular path or star graph. [17] discussed the ABS Estrada index of trees. [18] discussed the ABC index of chemical trees and its structural properties, focusing on trees with different degree sequences and specific vertex conditions. [19] introduced and examined the properties of the Laplacian ABC-matrix of graphs, focusing on its eigenvalues and their differences from those of standard Laplacian matrices. [20] introduced some useful graph transformations, and presented some properties of n-optimal trees. In recent years, the ABS index has become a research hotspot, which is obtained from the ABC index. Ali et al. in [21] contrasted the disparities between the ABC index and the ABS index. They demonstrated that for a graph satisfying $\delta \geq 2$, the value of the ABS index is invariably larger than that of the ABC index. Ali et al. in [22] conducted a comprehensive investigation of the ABS index of unicyclic graphs and their applications. Their work not only uncovered the inherent properties of the ABS index in the domain of unicyclic graphs but also expounded on its potential value for applications within this particular graph class. [23] studied the chemical significance of the ABS spectral radius and found that it is superior to the ABS index in predicting certain physicochemical properties of molecules. The reference [24] studies the spectral properties of matrices that depend on the ABS index, including the ABS-matrix, the Laplacian ABS-matrix, and the S_α matrix. [25] introduced the ABS index, and presented upper and lower bounds for this index in terms of graph parameters and other graph indices. [26] discussed the Sombor index of chemical graphs, characterizing these graphs based on this index across different molecular structures such as connected chemical graphs, chemical trees, and hexagonal systems. [27] introduced extremal problems related to the Sombor index of unicyclic graphs with a specified diameter, extending previous work on trees to determine the maximum Sombor indices for such graphs. [28] explored the Sombor index, and evaluated its application across various graph transformations. [29] focused on graph theory's Sombor index, finding its limits and noting how cycle graph C_n minimizes it among certain graphs.

In this paper, we have obtained some results of ABS spectral radius, and combined with some properties of octane isomers, to conduct a series of studies on the ability of the ABS spectral radius to predict molecular properties. In Section 2, several lemmas are presented that lay the theoretical foundation for the subsequent proofs. In Section 3, we focus on the ABS spectral radius and explore several bounds applicable to the ABS spectral radius. and their properties in various graph classes (e.g., trees, unicyclic graphs, complete bipartite, etc.). In Section 4, by analyzing the correlation between the ABS spectral radius and the physicochemical properties of octane isomers, the predictive ability of

the spectral radius of ABS in the modeling of chemical structure activity is verified, and the potential application value of the spectral radius of ABS in the chemical field is demonstrated. In Section 5, ABS energy and its related properties are studied.

2. Preliminaries

Lemma 2.1. *Let $\rho_1(R(G))$ be the Randić spectral radius of a connected graph G. Then, $\rho_1(R(G)) = 1$.*

Lemma 2.2. *Let M_1 and M_2 be nonnegative $n\times n$ matrices. The notation $M_1 \preceq M_2$ denotes the element relation where $(M_1)_{ij} \geq (M_2)_{ij}$ for all indices i, j. If $M_1 \preceq M_2$, then for their spectral radius $\rho(M_1)$ and $\rho(M_2)$, the inequality $\rho(M_1) \leq \rho(M_2)$ holds. Moreover, when M_1 is irreducible, and $M_1 \neq M_2$, we can state that $\rho(M_1) < \rho(M_2)$.*

Lemma 2.3. *Let P be a nonnegative irreducible matrix. Denote by r the average of the row sums of P and by R the maximum row sum of P. Then, the spectral radius $\rho(P)$ satisfies the inequality $r \leq \rho(P) \leq R$. Moreover, equality in either bound holds if and only if all row sums of P are equal.*

Lemma 2.4. *Let M be a nonnegative irreducible matrix with an eigenvalue θ. Let $\alpha \in \mathbb{R}$ and a nonnegative vector $Y \in \mathbb{R}^n$. Suppose that $MY \leq \alpha Y$; it follows that $\theta \leq \alpha$.*

Lemma 2.5. *Let G be a graph and $n \geq 3$ without isolated vertices. Then, $S(G)$ has a single distinct eigenvalue if and only if n is even, and $G = \left(\frac{n}{2}\right) K_2$.*

Lemma 2.6. *Suppose M is an n-order nonnegative symmetric matrix, and it denotes the adjacency matrix of a connected graph. Denote by $\rho_1, \rho_2, \ldots, \rho_k$ the eigenvalues of matrix M for which $|\rho_i| = \rho(M)$ $(i = 1, 2, \ldots, k)$, where $\rho(M)$ denotes the spectral radius of M. Then, $k > 1$ if and only if the length of every closed walk in graph G is a multiple of k.*

Lemma 2.7. *Assuming that A is a nonsingular square matrix, then*

$$\det\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \det(A)\det(D - CA^{-1}B).$$

3. ABS spectral radius

Theorem 3.1. *Let G be a connected graph. Then,*

$$\min_{i\sim j} \sqrt{\frac{d_i d_j (d_i + d_j - 2)}{d_i + d_j}} \leq \rho(S(G)) \leq \max_{i\sim j} \sqrt{\frac{d_i d_j (d_i + d_j - 2)}{d_i + d_j}}; \tag{3.1}$$

the equality holds if and only if G is regular or bipartite regular.

Proof. If G is connected, then $R(G)$ and $S(G)$ are both nonnegative irreducible matrices. We have

$$\min_{i\sim j} \sqrt{\frac{d_i d_j (d_i + d_j - 2)}{d_i + d_j}} R(G) \leq \rho(S(G)) \leq \max_{i\sim j} \sqrt{\frac{d_i d_j (d_i + d_j - 2)}{d_i + d_j}} R(G). \tag{3.2}$$

By Lemmas 2.1 and 2.2, (3.1) can be derived.

Next, we will discuss the situation where the equality holds in (3.1). We assume that

$$\alpha = \min_{i\sim j} \sqrt{\frac{d_i d_j (d_i + d_j - 2)}{d_i + d_j}} \text{ and } \beta = \max_{i\sim j} \sqrt{\frac{d_i d_j (d_i + d_j - 2)}{d_i + d_j}}.$$

First, assume that $\rho(S(G)) = \alpha$. Then, from Eq (3.2) and Lemma 2.2, it follows that $S(G) = \alpha R(G)$. This equality implies that for all $v_i v_j \in E(G)$, the equation

$$\sqrt{\frac{d_i d_j (d_i + d_j - 2)}{d_i + d_j}} = \alpha$$

holds. Let v_i be a vertex with degree δ. Then,

$$\alpha = \sqrt{\frac{\delta d_j (d_j + \delta - 2)}{d_j + \delta}} \leq \sqrt{\frac{\delta \Delta (\Delta + \delta - 2)}{\Delta + \delta}}.$$

Let v_i be a vertex with degree Δ. Then,

$$\alpha = \sqrt{\frac{\Delta d_j (d_j + \Delta - 2)}{d_j + \Delta}} \geq \sqrt{\frac{\delta \Delta (\Delta + \delta - 2)}{\Delta + \delta}}.$$

Thus,

$$\alpha = \sqrt{\frac{\delta \Delta (\Delta + \delta - 2)}{\Delta + \delta}}.$$

In this case, every neighbor of a minimum degree vertex is a maximum degree vertex, and the reverse is also true; it follows that G is regular or bipartite semiregular. Likewise, the treatment of the situation in which $\rho(S(G)) = \beta$ is quite similar.

On the contrary, for all edges $v_i v_j \in E(G)$, when G is a regular graph or a bipartite semiregular graph, we have

$$\sqrt{\frac{d_i d_j (d_i + d_j - 2)}{d_i + d_j}} = \alpha = \beta\,;$$

then,

$$S(G) = \alpha R(G) = \beta R(G).$$

By the Lemma 2.1, we observe that $\rho(S(G)) = \alpha = \beta$. □

Corollary 3.2. *Let G be connected. Then,*

$$\sqrt{\delta(\delta - 1)} \leq \rho(S(G)) \leq \sqrt{\Delta(\Delta - 1)}.$$

If and only if G is a regular graph, the equalities for both inequalities are satisfied.

Theorem 3.3. *Let G be a triangle-free connected graph, and $n \geq 3$. Then,*

$$\rho(S(G)) \leq \frac{n}{2}\sqrt{1 - \frac{2}{n}},$$

there is equality if and only if $G \cong K_{\frac{n}{2},\frac{n}{2}}$.

Proof. Let G be triangle-free. For all $v_iv_j \in E(G)$, the set of the neighborhoods of v_i and v_j, denoted as $N_G(v_i)$ and $N_G(v_j)$, have an empty intersection; therefore, $N_G(v_i) \cap N_G(v_j) = \varnothing$. Moreover, in view of the fact that the union of the two neighborhoods is included in the vertex set of G, we obtain $\left|N_G(v_i) \cup N_G(v_j)\right| \leq n$, where $n = |V(G)|$. We then have

$$d_i + d_j = |N_G(v_i)| + |N_G(v_j)| = |N_G(v_i) \cup N_G(v_j)| + |N_G(v_i) \cap N_G(v_j)| \leq n.$$

By this inequality, we can infer that $d_id_j \leq \frac{n^2}{4}$. Therefore, by Theorem 3.1, we obtain

$$\rho(S(G)) \leq \max_{i\sim j} \sqrt{d_id_j - \frac{2d_id_j}{d_i + d_j}} \leq \sqrt{d_id_j - \frac{2d_id_j}{n}} \leq \frac{n}{2}\sqrt{1 - \frac{2}{n}}.$$

It is obvious that if $G \cong K_{\frac{n}{2},\frac{n}{2}}$, we have $\rho(S(G)) = \frac{n}{2}\sqrt{1 - \frac{2}{n}}$. Conversely, assuming that $\rho(S(G)) = \frac{n}{2}\sqrt{1 - \frac{2}{n}}$, all of the inequalities mentioned above must hold as equalities and G is either regular or bipartite semiregular. Next, we assume that

$$d_a + d_b = \max_{i\sim j}(d_i + d_j) = n.$$

As a result, every vertex within $N_G(v_a)$ has a degree of $d_b = |N_G(v_b)|$, and every vertex in $N_G(v_b)$ has a degree of $d_a = |N_G(v_a)|$. Furthermore, due to the fact that G is triangle-free, both $N_G(v_a)$ and $N_G(v_b)$ are independent sets. Consequently, every vertex in $N_G(v_a)$ has an edge to each vertex within $N_G(v_b)$, and symmetrically, each vertex in $N_G(v_b)$ has an edge to each vertex within $N_G(v_a)$. If $|N_G(v_a)|+|N_G(v_b)| = n$, we have $G \cong K_{\frac{n}{2},\frac{n}{2}}$. □

Theorem 3.4. *Let G be a unicyclic graph with n vertices. Then,*

$$\rho(S(G)) \geq \frac{4}{\Delta}\sqrt{\frac{\Delta - 1}{\Delta}},$$

equality holds if and only if $G \cong C_n$.

Proof. As G is a unicyclic graph which consists of n vertices, we have $\sum_{i=1}^{n} d_i = 2n$. By Lemma 2.3, we obtain

$$\begin{aligned}\rho(S(G)) &\geq \frac{2}{n}\sum_{i\sim j}\sqrt{\frac{d_i + d_j - 2}{d_i + d_j}} = \frac{2}{n}\sum_{i\sim j}\sqrt{\frac{d_i + d_j - 2}{(d_i + d_j)^3}}(d_i + d_j)\\ &\geq \frac{1}{n}\sqrt{\frac{\Delta - 1}{\Delta^3}}\sum_{i\sim j}(d_i + d_j) = \frac{1}{n}\sqrt{\frac{\Delta - 1}{\Delta^3}}\sum_{i=1}^{n} d_i^2.\end{aligned} \tag{3.3}$$

Using the Cauchy-Schwarz inequality, we can infer that $\left(\sum_{i=1}^{n} d_i\right)^2 \leq n\sum_{i=1}^{n} d_i^2$, where the equality holds if and only if $d_1 = d_2 = \cdots = d_n$. Thus,

$$\begin{aligned}\rho(S(G)) &\geq \frac{1}{n}\sqrt{\frac{\Delta - 1}{\Delta^3}}\sum_{i=1}^{n} d_i^2 \geq \frac{1}{n^2}\sqrt{\frac{\Delta - 1}{\Delta^3}}(\sum_{i=1}^{n} d_i)^2\\ &= \frac{1}{n^2}\sqrt{\frac{\Delta - 1}{\Delta^3}}4n^2 = 4\sqrt{\frac{\Delta - 1}{\Delta^3}} = \frac{4}{\Delta}\sqrt{\frac{\Delta - 1}{\Delta}}.\end{aligned} \tag{3.4}$$

If $G \cong C_n$, we have $\rho(S(G)) = \frac{4}{\Delta}\sqrt{\frac{\Delta-1}{\Delta}} = \sqrt{2}$. Conversely, if $\rho(S(G)) = \frac{4}{\Delta}\sqrt{\frac{\Delta-1}{\Delta}}$, then $d_i = 2, i = 1, 2, ..., n.$; that is, $G \cong C_n$. □

Corollary 3.5. *Let $l(G)$ be the length of the cycle present in the unicyclic graph G. If $l(G) = 3$, then*

$$\rho(S(G)) \leq \frac{4}{n-1}\sqrt{\frac{n-2}{n-1}}.$$

If $l(G) = 4$, then

$$\rho(S(G)) \leq \frac{4}{n-2}\sqrt{\frac{n-3}{n-2}}.$$

We can infer that $\Delta = n - l(G) - 2$; then,

$$\rho(S(G)) \leq \frac{4}{n-l(G)+2}\sqrt{\frac{n-l(G)+1}{n-l(G)+2}}.$$

In the same vein, we know that if $G \cong C_n$, then $\rho(S(G)) = \sqrt{2}$.

Theorem 3.6. *Let G be a unicyclic graph with n vertices. If $\gamma = \max\{d_i + d_j | i \sim j\} \leq n - 1$, then,*

$$\rho(S(G)) \leq \sqrt{\frac{(n-3)(n+1)}{n-1}}.$$

Proof. Let $Y = (\sqrt{d_1}, \sqrt{d_2}, \ldots, \sqrt{d_n})^T$. Because $\gamma \leq n - 1$, then $1 \leq d_i \leq n - 3,\ i = 1, 2, ..., n$. We can derive that

$$\sum_{v_j \in N(v_i)} d_j = 2n - d_i - \sum_{v_k \notin (N(v_i) \cup v_i)} d_k \leq 2n - d_i - \sum_{v_k \notin (N(v_i) \cup v_i)} 1 = n + 1.$$

$$(SY)_i = \sum_{i \sim j} \sqrt{1 - \frac{2}{d_i + d_j}}\sqrt{d_j} \leq \sqrt{1 - \frac{2}{n-1}} \sum_{i \sim j} \sqrt{d_j}.$$

By the Cauchy-Schwarz inequality, we have

$$\sum_{i \sim j} \sqrt{d_j} \leq \sqrt{\sum_{i \sim j} d_j}\sqrt{d_i} \leq \sqrt{n+1}\sqrt{d_i}.$$

Thus,

$$(SY)_i \leq \sqrt{1 - \frac{2}{n-1}}\sqrt{n+1}\sqrt{d_i},\ SY \leq \sqrt{1 - \frac{2}{n-1}}\sqrt{n+1}\, Y.$$

From Lemma 2.4, we can see that

$$\rho(S(G)) \leq \sqrt{1 - \frac{2}{n-1}}\sqrt{n+1} = \sqrt{\frac{(n-3)(n+1)}{n-1}}.$$

□

The following theorem has already been mentioned in [23], and another method is proposed here.

Theorem 3.7. *Let T be an n order tree. Then,*

$$\rho(S(T)) \leq \sqrt{\frac{(n-2)(n-1)}{n}}.$$

The above inequality holds if and only if $T \cong S_n$.

Proof. For every edge $v_kv_i \in E(G)$, we have $d_i + d_k \leq n$. Let m_i be the average degree of neighbors of v_i. For any $v_i \in V(T)$, it holds that $d_i + m_i \leq d_i + \frac{n-1}{d_i} \leq n$ ($d_i \leq n-1$); thus, $d_km_k \leq n-1$ for any $v_k \in V(T)$.

Let $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$ be the eigenvector corresponding to $\rho(S(T))$ of $S(T)$, that is, $S(T)\mathbf{x} = \rho(S(T))\mathbf{x}$. Let $x_k = 1$, $|x_j| \leq 1$. Then, for $v_i \in V(T)$, we have

$$\rho(S(T))x_i = \sum_{v_j \in N(v_i)} \sqrt{1 - \frac{2}{d_i + d_j}}\, x_j.$$

For $v_k \in V(T)$, we have

$$\rho(S(T)) = \sum_{v_i \in N(v_k)} \sqrt{1 - \frac{2}{d_i + d_k}}\, x_i.$$

Thus,

$$\begin{aligned}
\rho(S(T))^2 &= \sum_{v_i \in N(v_k)} \sqrt{1 - \frac{2}{d_i + d_k}}\, x_i \\
&= \sum_{v_i \in N(v_k)} \sqrt{1 - \frac{2}{d_i + d_k}} \sum_{v_j \in N(v_i)} \sqrt{1 - \frac{2}{d_i + d_j}}\, x_j \\
&\leq \sum_{v_i \in N(v_k)} \sqrt{1 - \frac{2}{d_i + d_k}} \sum_{v_j \in N(v_i)} \sqrt{1 - \frac{2}{d_i + d_j}} \\
&= \sum_{v_i \in N(v_k)} \sqrt{1 - \frac{2}{d_i + d_k}}\, d_i \sqrt{1 - \frac{2}{d_i + m_i}} \\
&\leq (1 - \frac{2}{n}) \sum_{v_i \in N(v_k)} d_i = (1 - \frac{2}{n}) d_k m_k \leq (1 - \frac{2}{n})(n-1).
\end{aligned} \tag{3.5}$$

We can conclude that

$$\rho(S(T)) \leq \sqrt{(1 - \frac{2}{n})(n-1)} = \sqrt{\frac{(n-2)(n-1)}{n}}.$$

If the equality holds, then $d_k + d_i = n$ for all $v_iv_k \in E(T)$. We can infer that $d_i + m_i = n$ for all $v_i \in N(v_k)$, and $d_km_k = n-1$ for all $v_k \in V(T)$. For $v_i \in V(T)$, $d_i + m_i = d_i + \frac{n-1}{d_i} = n$ if and only if $d_i = 1$ or $d_i = n-1$, that is, $T \cong S_n$.

Conversely, if $T \cong S_n$, we have

$$S(T) = \sqrt{\frac{n-2}{n}} A(T);$$

therefore,

$$\rho(S(T)) = \sqrt{\frac{n-2}{n}}\sqrt{\frac{n(n-1)}{n}} = \sqrt{\frac{(n-2)(n-1)}{n}}.$$

□

Theorem 3.8. *Let P_n be a path with n vertices. Then, $-2\sqrt{\frac{1}{2}} < \rho_i(P_n) < 2\sqrt{\frac{1}{2}}$ for $1 \le i \le n$.*

Proof. Let $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$ be the eigenvector corresponding to ρ_i of $S(P_n)$. Let $x_p = 1$, $|x_q| = 1$, and $1 \le q \le n$. We have $S(P_n)\mathbf{x} = \rho_i(P_n)\mathbf{x}$, which implies

$$\begin{cases} \rho_i(P_n)x_1 = \sqrt{\frac{1}{3}}x_2 \\ \rho_i(P_n)x_2 = \sqrt{\frac{1}{3}}x_1 + \sqrt{\frac{1}{2}}x_3 \\ \rho_i(P_n)x_j = \sqrt{\frac{1}{2}}x_{j-1} + \sqrt{\frac{1}{2}}x_{j+1} \quad \text{for } 3 \le j \le n-2 \\ \rho_i(P_n)x_{n-1} = \sqrt{\frac{1}{2}}x_{n-2} + \sqrt{\frac{1}{3}}x_n \\ \rho_i(P_n)x_n = \sqrt{\frac{1}{3}}x_{n-1}. \end{cases}$$

Let the vertex set $S = \{v_1, v_2, v_{n-1}, v_n\}$. If $v_p \in S$, then from the above equations, we have:

$$\rho_i(P_n) = \rho_i(P_n)x_p < 2\sqrt{\frac{1}{2}} \quad \text{and} \quad \rho_i(P_n) = \rho_i(P_n)x_p > -2\sqrt{\frac{1}{2}}.$$

If $x_p \in V(P_n) \setminus S$, we set $x_i < 1$ for $i = 1, 2, n-1, n$. From the above equations, we obtain

$$\rho_i(P_n) = \rho_i(P_n)x_p = \sqrt{\frac{1}{2}}x_{p-1} + \sqrt{\frac{1}{2}}x_{p+1} \le 2\sqrt{\frac{1}{2}},$$

and similarly,

$$\rho_i(P_n) = \rho_i(P_n)x_p = \sqrt{\frac{1}{2}}x_{p-1} + \sqrt{\frac{1}{2}}x_{p+1} \ge -2\sqrt{\frac{1}{2}}.$$

Conversely, we prove that $\rho_i(P_n) < 2\sqrt{\frac{1}{2}}$. Let $\rho_i(P_n) < 2\sqrt{\frac{1}{2}}$. Then, we have $x_{p-1} = x_{p+1} = 1$. Similarly, for $x_p + 1 \in V(P_n) \setminus S$, we have

$$\rho_i(P_n) = \rho_i(P_n)x_{p+1} = \sqrt{\frac{1}{2}}x_p + \sqrt{\frac{1}{2}}x_{p+2};$$

therefore, $x_{p+2} = 1$. Repeating the process, we obtain $x_2 = x_3 = \cdots = x_p = \cdots = x_{n-1} = 1$, which leads to a contradiction. Likewise, we can show that $\rho_i(P_n) > -2\sqrt{\frac{1}{2}}$. □

4. Correlation analysis between octane isomers and ABS spectral radius

In addition to mathematical exploration, establishing chemical connections with graph invariants represents a contemporary research trend within the realm of computational graph theory. Randić and Trinajstić proposed several components for probing into the practical application value of graph

invariants. In order to assess the predictive capacity of an index, it is necessary to establish a correlation between the theoretical values of indices and the experimental properties of a benchmark data set. The chemical graphs associated with octane isomers are in the form of trees. These trees have eight vertices, and for each vertex, the maximum degree is at most four. In chemical graph theory, a "chemical tree" is a tree-graph model used to represent the topological structure of organic molecular skeletons. Its fundamental conventions are that vertices correspond to nonhydrogen atoms in the molecule (such as carbon atoms), edges correspond to chemical bonds between atoms, and hydrogen atoms are typically omitted. Figure 1 shows the chemical trees of the octane isomers considered in this paper.

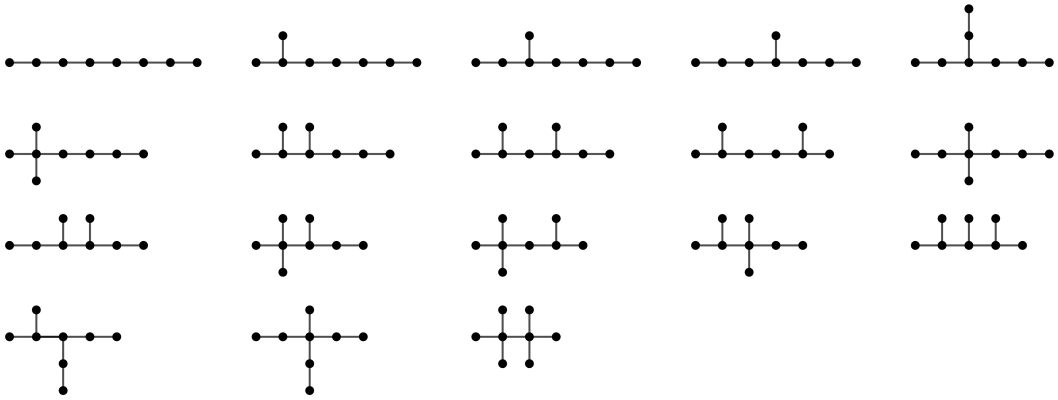


Figure 1. Chemical tree of octane isomers.

In chemoinformatics and drug design, molecular descriptors play a crucial role in establishing quantitative structure–property/activity relationship (QSPR/QSAR) models. Among them, Voronoi diagram analysis(VDA) accurately describes the three-dimensional surface shape of molecules through geometric partitioning; Shape matching target intermolecular (SMTI) quantifies the degree of shape complementarity between a molecule and its biological target; Geometric moment topological index (GMTI) serves as a comprehensive descriptor integrating the three-dimensional shape and two-dimensional topological structure of molecules; and Hydrophobic distribution profile (HyDp) characterizes the spatial distribution of hydrophobicity on the molecular surface. Collectively, these descriptors digitally represent the interaction mechanisms between molecules and biological targets from multiple dimensions, including geometric matching, topological structure, and chemical property distribution. By analyzing the correlation between the ABS spectral radius of octane isomers and the aforementioned descriptors, this study aims to validate the potential and application value of the ABS spectral radius in predicting complex molecular properties. Complete experimental data on the physicochemical properties of octane isomers are available at: `https://web.archive.org/web/20170712072219/http://www.moleculardescriptors.eu/dataset/c8.rar`.

The ABS spectral radius of the chemical trees in Figure 1 and several properties of octane isomers are shown in Table 1. The approximate values of correlation coefficients between the VDA, SMTI, GMTI, and HyDp of octane isomers and ABS spectral radius and ABC spectral radius can be obtained by calculation, which are shown in Table 2. One can observe that the ABS spectral radius is more effective than the ABC spectral radius in predicting the VDA, SMTI, GMTI, and HyDp of octane

isomers. Table 2 also indicates that the ABS spectral radius is a good predictive indicator for the VDA, SMTI, GMTI, and HyDp of octane isomers. This shows that it is reasonable to introduce ABS spectral radius as a prediction parameter in chemistry. The values of spectral radius in Tables 1 and 2 were calculated by MATLAB.

Table 1. Experimental data of VDA, SMTI, GMTI, HyDp, $\rho_{ABS}(S)$, $\rho_{ABC}(S)$ octane isomers.

Molecule	**VDA**	**SMTI**	**GMTI**	**HyDp**	$\rho_{ABS}(S)$	$\rho_{ABC}(S)$
octane	21	306	231	210	1.3076	1.3289
2-methyl-heptane	19.75	288	211	185	1.4102	1.4541
3-methyl-heptane	19	276	199	170	1.4520	1.4462
4-methyl-heptane	18.75	272	195	165	1.4677	1.4543
3-ethyl-hexane	18	260	183	150	1.4922	1.4344
2,2-dimethyl-hexane	17.75	260	179	149	1.6354	1.7000
2,3-dimethyl-hexane	17.5	254	175	143	1.5568	1.5386
2,4-dimethyl-hexane	17.75	258	179	147	1.5195	1.5228
2,5-dimethyl-hexane	18.5	270	191	161	1.4687	1.5082
3,3-dimethyl-hexane	16.75	244	163	131	1.6714	1.6594
3,4-dimethyl-hexane	17	246	167	134	1.5744	1.5229
2-methyl-3-ethyl-pentane	16.75	242	163	129	1.5802	1.5231
3-methyl-3-ethyl-pentane	16	232	151	118	1.6922	1.6143
2,2,3-trimethyl-pentane	15.75	230	147	115	1.7262	1.7251
2,2,4-trimethyl-pentane	16.5	242	159	127	1.6733	1.7234
2,3,3-trimethyl-pentane	15.5	226	143	111	1.7372	1.6973
2,3,4-trimethyl-pentane	16.25	236	155	122	1.6261	1.5933
2,2,3,3-tetramethylbutane	14.5	214	127	97	1.8428	1.8371

Table 2. The correlation coefficient of VDA, SMTI, GMTI, and HyDp of octane isomers with $\rho_{ABS}(S)$ and $\rho_{ABC}(S)$.

Property	$\rho_{ABS}(S)$	$\rho_{ABC}(S)$
VDA	-0.9662	-0.8660
SMTI	-0.9543	-0.8402
GMTI	-0.9663	-0.8660
HyDp	-0.9524	-0.8434

Next, three types of regression models are studied, which include linear, quadratic, and cubic. Here are the three regression models.

$$y = a + b_1 x_1; \quad n, R \text{ (Linear)} \tag{4.1}$$

$$y = a + b_1 x_2 + b_2 x_2^2; \quad n, R \text{ (Quadratic)} \tag{4.2}$$

$$y = a + b_1 x_3 + b_2 x_3^2 + b_3 x_3^3; \quad n, R \text{ (Cubic)}. \tag{4.3}$$

Let y denote the dependent variable, a be the regression constant, and b_i (where $i = 1, 2, 3$) be the regression coefficients. The variables x_i are the independent variables. The samples are used in the

formulation of the regression equation. Here, the correlation coefficient is denoted by R, the standard error of the estimates is denoted by SE, and Fisher's statistic is represented as F.

The linear regression models are as follows:

$$\begin{aligned}
\text{VDA} &= -11.6994 \cdot \rho_{\text{ABS}} + 35.7910, \quad R^2 = 0.9337,\\
\text{SMTI} &= -165.5314 \cdot \rho_{\text{ABS}} + 514.5946, \quad R^2 = 0.9106,\\
\text{GMTI} &= -186.3909 \cdot \rho_{\text{ABS}} + 467.6567, \quad R^2 = 0.9337,\\
\text{HyDp} &= -200.3224 \cdot \rho_{\text{ABS}} + 458.8859, \quad R^2 = 0.9071.
\end{aligned}$$

The quadratic regression models are as follows:

$$\begin{aligned}
\text{VDA} &= 7.3885 \cdot \rho_{\text{ABS}}^2 - 34.9344 \cdot \rho_{\text{ABS}} + 54.0188, \quad R^2 = 0.9434,\\
\text{SMTI} &= 140.1581 \cdot \rho_{\text{ABS}}^2 - 607.3369 \cdot \rho_{\text{ABS}} + 860.3715, \quad R^2 = 0.9275,\\
\text{GMTI} &= 118.2161 \cdot \rho_{\text{ABS}}^2 - 559.0307 \cdot \rho_{\text{ABS}} + 759.3010, \quad R^2 = 0.9434,\\
\text{HyDp} &= 219.6087 \cdot \rho_{\text{ABS}}^2 - 892.5713 \cdot \rho_{\text{ABS}} + 1000.6711, \quad R^2 = 0.9353.
\end{aligned}$$

The cubic regression models are as follows:

$$\begin{aligned}
\text{VDA} &= -25.5799 \cdot \rho_{\text{ABS}}^3 + 128.2397 \cdot \rho_{\text{ABS}}^2 - 224.1620 \cdot \rho_{\text{ABS}} + 152.1861,\\
R^2 &= 0.9468,\\
\text{SMTI} &= -361.5460 \cdot \rho_{\text{ABS}}^3 + 18498.2605 \cdot \rho_{\text{ABS}}^2 - 3281.7949 \cdot \rho_{\text{ABS}} + 2249.0012,\\
R^2 &= 0.9308,\\
\text{GMTI} &= -409.2779 \cdot \rho_{\text{ABS}}^3 + 7051.8360 \cdot \rho_{\text{ABS}}^2 - 3586.5933 \cdot \rho_{\text{ABS}} + 2330.1372,\\
R^2 &= 0.9468,\\
\text{HyDp} &= -534.5696 \cdot \rho_{\text{ABS}}^3 + 2749.1649 \cdot \rho_{\text{ABS}}^2 - 4846.9560 \cdot \rho_{\text{ABS}} + 3032.3946,\\
R^2 &= 0.9402.
\end{aligned}$$

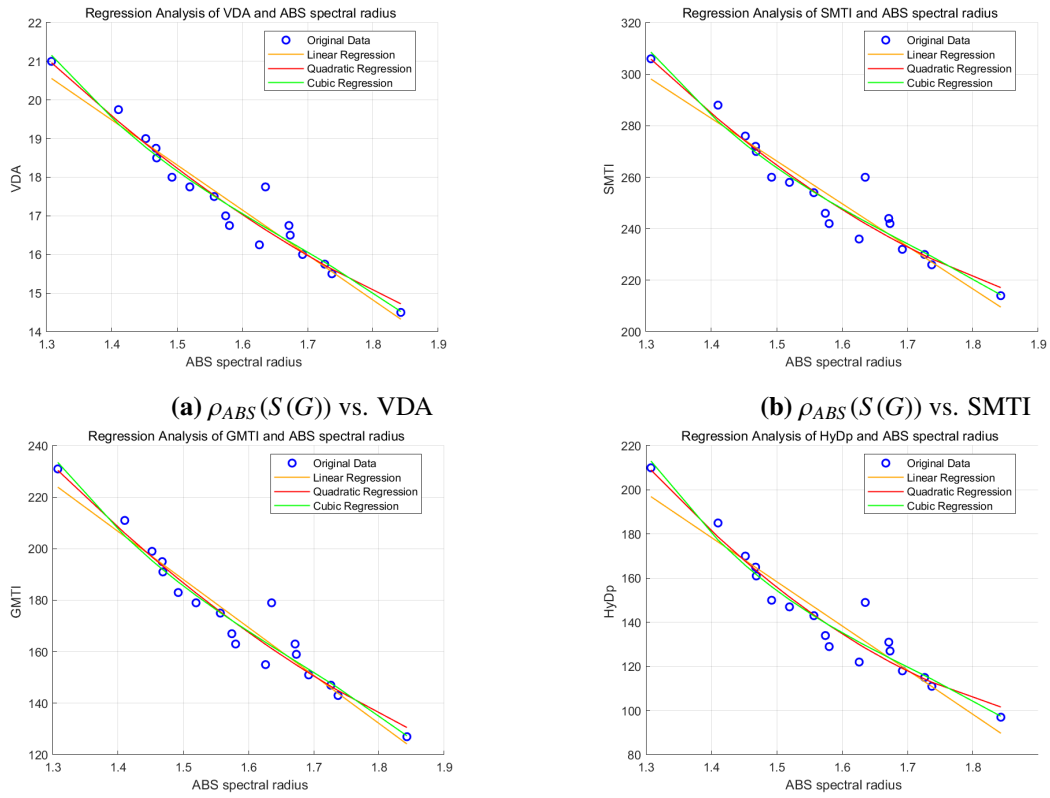
The correlation between VDA, SMTI, GMTI, HyDp, and ABS spectral radius is shown in Figure 2. In each subplot of Figure 2, the points (x, y) correspond to the ABS spectral radius and a physicochemical property of the octane isomers, respectively. The curves represent the fitted regression lines.

The root mean square error (RMSE) is a key metric for evaluating prediction accuracy. By accurately measuring the differences between observed and true values, it provides a rigorous basis for assessing how accurately a model fits the data in a mathematical context. In model assessment, the relationship between RMSE values and model performance is distinctly negative and significant. A lower RMSE means a better fit and higher predictive reliability, whereas a higher RMSE indicates significant deviations. The RMSE is defined as:

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{n}},$$

where n denotes the quantity of samples, y_i is the true value of the i-data point, and $\hat{y}_i$ is the predicted value of the i-data point. It is observed from the above data that, in all the regression models considered

for the ABS spectral radius, the potentially best predictive index for VDA is tabulated in Table 3. It is readily apparent from Table 3 that in all cases, the RMSE value is the smallest for ABS, and the coefficient of determination (R^2) is closer to 1, which proves that the ABS spectral radius is a good predictor.



(a) $\rho_{ABS}(S(G))$ vs. VDA

(b) $\rho_{ABS}(S(G))$ vs. SMTI

(c) $\rho_{ABS}(S(G))$ vs. GMTI

(d) $\rho_{ABS}(S(G))$ vs. HyDp

Figure 2. Scatter plots of ABS spectral radius with various molecular descriptors.

Table 3. Statistical parameters of different regression models for ABS spectral radius and VDA.

	R^2	F	SE	RMSE
Linear	0.9337	225.1933	0.4168	0.4051
Quadratic	0.9434	124.9284	0.3852	0.3743
Cubic	0.9468	83.0238	0.3734	0.3628

5. ABS energy

For graph G, the ABS energy $E_{ABS}(G)$ is obtained by summing up the absolute values of all ABS eigenvalues of graph G.

Proposition 5.1. *Let* $G = G_1 \cup G_2 \cup G_3 \cup \cdots \cup G_p$. *Then,*

$$E_{ABS}(G) = E_{ABS}(G_1) + E_{ABS}(G_2) + \cdots + E_{ABS}(G_p).$$

The ABS eigenvalues of a graph are the result of combining the eigenvalues of each of the components of the graph.

Proposition 5.2. *Let G be a graph with the order $n \geq 3$ and without isolated vertices.*

(i) If G is a r-regular graph, and $r \geq 2$, we obtain

$$E_{ABS}(G) = \sqrt{\frac{r-1}{r}} E(G).$$

If $r = 0$ or 1, then $E_{ABS}(G) = 0$. In particular,

$$E_{ABS}(K_n) = 2\sqrt{(n-2)(n-1)}.$$

(ii) If G is an (r, s)-semiregular bipartite graph, then $E_{ABS}(G) = \sqrt{\frac{r+s-2}{r+s}} E(G)$. Subsequently, we can also deduce

$$E_{ABS}(K_{a,b}) = 2\sqrt{\frac{n-2}{n}}\sqrt{ab} \leq 2\sqrt{\frac{n-2}{n}}\frac{n}{2} = \sqrt{n(n-2)},$$

(where $a + b = n$).

The harmonic index [30] is

$$H(G) = \sum_{v_i v_j \in E(G)} \frac{2}{d_i + d_j}.$$

Proposition 5.3. *Let G be a graph of order $n \geq 3$ with no isolated vertices. Then,*

$$E_{ABS}(G) \geq 2\sqrt{m - H(G)}.$$

Equality holds if and only if $G = \left(\frac{n}{2}\right) K_2$ or $n - a - b$ is even, and $G = \frac{n-a-b}{2} K_2 \cup K_{a,b}$, where $a + b \geq 3$.

Proof. It is known that

$$\sum_{i=1}^{n} \rho_i(G) = 0, \quad \sum_{i=1}^{n} \rho_i^2(G) = 2(m - H(G)), \quad H(G) = \frac{2}{n} \sum_{i<j} \frac{1}{d_i + d_j}.$$

We have

$$\begin{aligned} E_{ABS}(G)^2 &= \sum_{i=1}^{n} |\rho_i(G)|^2 + 2 \sum_{1 \leq i < j \leq n} |\rho_i(G)\rho_j(G)| \\ &\geq \sum_{i=1}^{n} |\rho_i(G)|^2 + 2 \left| \sum_{i=1}^{n} \rho_i(G)\rho_j(G) \right| \\ &= 2(m - H(G)) + 2|H(G) - m| \\ &= 4(m - H(G)). \end{aligned} \tag{5.1}$$

Hence, $E_{ABS}(G) \geq 2\sqrt{m - H(G)}$.

If $E_{ABS}(G) = 2\sqrt{m - H(G)}$, because $\sum_{i=1}^{n} \rho_i(G) = 0$, it follows that $\rho_1(S(G)) = \cdots = \rho_n(S(G)) = 0$, or $\rho_1(S(G)) = -\rho_n(S(G)) \neq 0$, and $\rho_2(S(G)) = \cdots = \rho_{n-1}(S(G)) = 0$. For the first case, by Lemma 2.5,

we know that n is even, and $G = \frac{n}{2}K_2$. For the second case, according to Lemma 2.6, we can see that all closed walks in G have lengths that are multiples of k, which means that G is a bipartite graph.

Additionally, we find that G has a bipartite connected component C', $|V(C')| \geq 3$. G has three distinct eigenvalues, and C' does, as well; otherwise, we would have $C' = \frac{n}{2}K_2$ or $C' = K_n$, a contradiction. Therefore, $C' = K_{a,b}$, $a + b = n' \geq 3$, $n - a - b$ is even, and $G = \frac{n-a-b}{2}K_2 \cup K_{a,b}$.

Conversely, if n is even, and $G = \frac{n}{2}K_2$, or $n - a - b$ is even, and $G = \frac{n-a-b}{2}K_2 \cup K_{a,b}$, it is easy to derive that $E_{ABS}(G) = 2\sqrt{m - H(G)}$. □

Theorem 5.4. *For $n \geq 2$, the following two conclusions can be obtained.*

(i) The ABS characteristic polynomial of $S_n = K_{1,n-1}$ is

$$\varphi_{ABS}(S_n, \rho) = \rho^{n-2}(\rho^2 - \frac{(n-2)(n-1)}{n}).$$

(ii) The ABS energy of S_n is

$$E_{ABS}(S_n) = 2\sqrt{\frac{(n-2)(n-1)}{n}}.$$

Proof. (i) We know that $S(K_{1,n-1})$ is

$$S(K_{1,n-1}) = S(S_n) = \sqrt{\frac{n-2}{n}}\begin{pmatrix} 0_{1\times 1} & \mathbf{J}_{1\times(n-1)} \\ \mathbf{J}_{(n-1)\times 1} & \mathbf{0}_{(n-1)\times(n-1)} \end{pmatrix}.$$

Then,

$$\det(\rho I - S(S_n)) = \det\begin{pmatrix} \rho & -\sqrt{\frac{n-2}{n}}\mathbf{J}_{1\times(n-1)} \\ -\sqrt{\frac{n-2}{n}}\mathbf{J}_{(n-1)\times 1} & \rho I_{n-1} \end{pmatrix}.$$

By Lemma2.7, we have

$$\det(\rho I - S(S_n)) = \rho det(\rho I_{n-1} - \sqrt{\frac{n-2}{n}}J_{(n-1)\times 1}\frac{1}{\rho}(\sqrt{\frac{n-2}{n}}J_{1\times(n-1)})).$$

Therefore,

$$\begin{aligned}\det(\rho I - S(S_n)) &= \rho \det\left(\rho I_{n-1} - \frac{1}{\rho}\frac{n-2}{n}J_{n-1}\right) \\ &= \rho^{2-n}\det\left(\rho^2 I_{n-1} - \frac{n-2}{n}J_{n-1}\right).\end{aligned}$$

And we know that the eigenvalues of J_{n-1} are $n-1, 0, 0, \ldots, 0$, so

$$\varphi_{\mathrm{ABS}}(S_n, \rho) = \rho^{n-2}(\rho^2 - \frac{(n-2)(n-1)}{n}).$$

(ii) From (i), we conclude that the eigenvalues of the matrix $S(S_n)$ are $\sqrt{\frac{(n-2)(n-1)}{n}}, -\sqrt{\frac{(n-2)(n-1)}{n}}, 0, 0, \ldots, 0$. By our definition of energy, we have

$$E_{ABS}(S_n) = 2\sqrt{\frac{(n-2)(n-1)}{n}}.$$

□

It can be seen from [23] that the unicyclic graph with the largest spectral radius is shown in Figure 3.

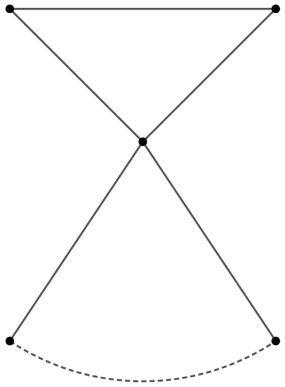


Figure 3. unicyclic graph U.

Corollary 5.5. *For the star graph S_n, connecting two pendant vertices yields a unicyclic graph U, so*

$$E_{ABS}(U) > E_{ABS}(S_n) = 2\sqrt{\frac{(n-2)(n-1)}{n}}.$$

Proof. By Theorem 5.4, we know that the eigenvalues of $S(S_n)$ are $\sqrt{\frac{(n-2)(n-1)}{n}}$, $-\sqrt{\frac{(n-2)(n-1)}{n}}$, $0, \cdots, 0$. Because U is derived from adding an edge to the star graph S_n, by the Courant-Fisher theorem, we have $\rho(S_n) < \rho(U_n)$. We have the matrix

$$B = \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ 0 & 1 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 \end{pmatrix},$$

and we have

$$\mathrm{tr}(S(S_n) + B) = \mathrm{tr}(S(S_n)) + \mathrm{tr}(B) = 0.$$

In summary, an increase in the spectral radius is accompanied by a decrease in the other eigenvalues. Consequently, the sum of the absolute values of the zero and negative eigenvalues increases. Therefore,

$$E_{ABS}(U) > E_{ABS}(S_n)2\sqrt{\frac{(n-2)(n-1)}{n}}.$$

□

Theorem 5.6. *Let $m, n \neq 1$ and $K_{m,n}$ be a complete bipartite graph.*

(i) The ABS characteristic polynomial of $K_{m,n}$ is

$$\varphi_{ABS}(K_{m,n}, \rho) = \rho^{m+n-2}(\rho^2 - mn\frac{m+n-2}{m+n}).$$

(ii) The ABS energy of $K_{m,n}$ is

$$E_{ABS}(K_{m,n}) = 2(m+n)\sqrt{mn\frac{m+n-2}{m+n}}.$$

Proof. (i) The ABS matrix of $K_{m,n}$ is

$$S(K_{m,n}) = \sqrt{\frac{m+n-2}{m+n}}\begin{pmatrix} 0_{m\times m} & \mathbf{J}_{m\times n} \\ \mathbf{J}_{n\times m} & \mathbf{0}_{n\times n} \end{pmatrix}.$$

We have

$$\det(\rho I - S(K_{m,n})) = \det\begin{pmatrix} \rho I_m & -\sqrt{\frac{m+n-2}{m+n}}\mathbf{J}_{m\times n} \\ -\sqrt{\frac{m+n-2}{m+n}}\mathbf{J}_{n\times m} & \rho I_n \end{pmatrix}.$$

Then, by Lemma 2.7,

$$\det(\rho I - S(K_{m,n})) = \rho det(\rho I_n - \sqrt{\frac{m+n-2}{m+n}}J_{n\times m}\frac{1}{\rho}I_m(\sqrt{\frac{m+n-2}{m+n}}J_{m\times n})).$$

Therefore,

$$\begin{aligned}\det(\rho I - S(K_{m,n})) &= \rho^m \det\left(\rho I_n - \frac{1}{\rho}m\frac{m+n-2}{m+n}J_{n-1}\right) \\ &= \rho^{m-n}\det\left(\rho^2 I_n - m\frac{m+n-2}{m+n}J_n\right).\end{aligned}$$

We know that the eigenvalues of J_n are $n, 0, 0, \ldots, 0$, so

$$\varphi_{\mathrm{ABS}}(K_{m,n}, \rho) = \rho^{m+n-2}(\rho^2 - mn\frac{m+n-2}{m+n}).$$

(ii) It follows from Part (i).

□

Similarly to the ABS spectral radius, ABS energy also finds applications in the field of chemistry. In [31], the physicochemical properties of benzenes were shown. It demonstrated that the boiling point and π-electron energy could be modeled by employing ABS energy, thus revealing the applicability of ABS energy in the field of chemistry.

6. Conclusions

This paper is dedicated to exploring the spectrum of the ABS index. First, the bound of the ABS spectral radius is clarified and the characteristics of ABS spectral radius are explored for several common types of graph. Using the octane isomer as the starting point, the correlation between the ABS spectral radius and the physicochemical properties, was analyzed extensively using linear, quadratic, and cubic regression models. The correlation between the ABS spectral radius and these physicochemical properties was confirmed to be substantially significant. Our analysis demonstrates that the ABS index exhibits superior performance compared to the ABC index in predicting the physicochemical properties of the studied molecules. Additionally, the ABS energy was methodically analyzed, revealing a profound relationship between the ABS energy and graph structure. Future research could explore the application of ABS spectral radius and energy in other fields, such as material science and bioinformatics, to further validate its versatility.

Author contributions

Xiangyu Ren: Conceptualization, Methodology, Project Administration; Jiangtong Liu: Conceptualization, Methodology, Data curation, Formal analysis, Software, Visualization, Writing-original draft. All authors have read and approved the final version of the manuscript for publication.

Use of Generative-AI tools declaration

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

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Conflict of interest

The authors hereby declare that, to the best of their knowledge, there are no competing financial interests or personal relationships that could potentially bias or influence the findings and presentation of the work reported in this paper.

References

1. M. Karelson, V. S. Lobanov, A. R. Katritzky, Quantum-chemical descriptors in qsar/qspr studies, *Chem. Rev.*, **96** (1996), 1027–1044. https://doi.org/10.1021/cr950202r
2. K. Varmuza, M. Dehmer, D. Bonchev, *Statistical Modelling of Molecular Descriptors in QSAR/QSPR*, Hoboken: Wiley Online Library, 2012.
3. I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. total φ-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.*, **17** (1972), 535–538. https://doi.org/10.1016/0009-2614(72)85099-1
4. K. C. Das, I. Gutman, I. Milovanović, E. Milovanović, B. Furtula, Degree-based energies of graphs, *Linear Algebra Appl.*, **554** (2018), 185–204. https://doi.org/10.1016/j.laa.2018.05.027
5. M. Randic, Characterization of molecular branching, *J. Am. Chem. Soc.*, **97** (1975), 6609–6615. https://doi.org/10.1021/ja00856a001
6. I. Gutman, B. Furtula, Recent results in the theory of randic index, Univ, *Kragujevac, Kragujevac*, 2008.
7. E. Estrada, L. Torres, L. Rodriguez, I. Gutman, An atom-bond connectivity index: Modelling the enthalpy of formation of alkanes, *Indian J. Chem. Sec. A: Inorg. Phys. Theor. Anal.*, **37** (1998), 849–855.

8. B. Zhou, N. Trinajstić, On a novel connectivity index, *J. Math. Chem.*, **46** (2009), 1252–1270. https://doi.org/10.1007/s10910-008-9515-z

9. A. Ali, B. Furtula, I. Redžepović, I. Gutman, Atom-bond sum-connectivity index, *J. Math. Chem.*, **60** (2022), 2081–2093. https://doi.org/10.1007/s10910-022-01403-1

10. A. Ali, M. Javaid, M. Matejić, I. Milovanović, E. Milovanović, Some new bounds on the general sum-connectivity index, *Commun. Comb. Optim.*, **5** (2020), 97–109. https://doi.org/10.22049/CCO.2019.26618.1125

11. X. Chen, On abc eigenvalues and abc energy, *Linear Algebra Appl.*, **544** (2018), 141–157. https://doi.org/10.1016/j.laa.2018.01.011

12. K. C. Das, S. Elumalai, I. Gutman, On abc index of graphs, *MATCH Commun. Math. Comput. Chem.*, **78** (2017), 459–468.

13. M. Goubko, C. Magnant, P. S. Nowbandegani, I. Gutman, Abc index of trees with fixed number of leaves, *MATCH Commun. Math. Comput. Chem*, **74** (2015), 697–702.

14. 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. https://doi.org/10.47443/dml.2020.0069

15. T. S. Vassilev, L. J. Huntington, On the minimum abc index of chemical trees, *Appl. Math.*, **2** (2012), 8–16. https://doi.org/10.5923/j.am.20120201.02

16. X. Chen, On extremality of abc spectral radius of a tree, *Linear Algebra Appl.*, **564** (2018), 159–169. https://doi.org/10.1016/j.laa.2018.12.003

17. Z. Lin, T. Zhou, Y. Liu, On abs estrada index of trees, *J. Appl. Math. Comput.*, **70** (2024), 5483–5495. https://doi.org/10.1007/s12190-024-02188-z

18. X. Wu, L. Zhang, On structural properties of abc-minimal chemical trees, *Appl. Math. Comput.*, **362** (2019), 124570. https://doi.org/10.1016/j.amc.2019.124570

19. N. Yang, B. Deng, X. Li, Laplacian abc-eigenvalues of graphs, *MATCH Commun. Math. Comput. Chem*, **85** (2021), 195–206.

20. Y. Gao, Y. Shao, The smallest abc index of trees with n pendent vertices, *MATCH Commun. Math. Comput. Chem*, **76** (2016), 141–158.

21. K. J. Gowtham, I. Gutman, On the difference between atom-bond sum-connectivity and sum-connectivity indices, *Bulletin*, **47** (2022), 55–66.

22. A. Ali, I. Gutman, I. Redžepović, Atom-bond sum-connectivity index of unicyclic graphs and some applications, *Electron. J. Math.*, **5** (2023), 1–7. https://doi.org/10.47443/ejm.2022.039

23. Z. Lin, Y. Liu, T. Zhou, On the atom-bond sum-connectivity spectral radius of trees, *Discrete Math. Lett.*, **13** (2024), 122–127. https://doi.org/10.47443/dml.2024.100

24. J. Liu, Y. Hu, X. Ren, Spectral properties of the atom-bond sum-connectivity matrix, *Contrib. Math.*, **10** (2024), 1–10. https://doi.org/10.47443/cm.2024.041

25. A. Jahanbani, I. Redžepović, On the generalized ABS index of graphs, *Filomat*, **37** (2023), 10161–10169.

26. R. Cruz, I. Gutman, J. Rada, Sombor index of chemical graphs, *Appl. Math. Comput.*, **399** (2021), 126018. https://doi.org/10.1016/j.amc.2021.126018

27. H. Liu, Extremal problems on sombor indices of unicyclic graphs with a given diameter, *Comput. Appl. Math.*, **41** (2022), 138. https://doi.org/10.1007/s40314-022-01852-z

28. H. S. Ramane, I. Gutman, K. Bhajantri, D. V. Kitturmath, Sombor index of some graph transformations, *Commun. Combin. Optim.*, **8** (2023), 193–205. https://doi.org/10.22049/CCO.2021.27484.1272

29. T. Réti, T. Došlic, A. Ali, On the sombor index of graphs, *Contrib. Math.*, **3** (2021), 11–18. https://doi.org/10.47443/cm.2021.0006

30. L. Zhong, The harmonic index for graphs, *Appl. Math. Lett.*, **25** (2012), 561–566. https://doi.org/10.1016/j.aml.2011.09.059

31. I. Gutman, The energy of a graph: Old and new results, In: *Algebraic Combinatorics and Applications: Proceedings of the Euroconference, Algebraic Combinatorics and Applications (ALCOMA), held in Gößweinstein, Germany, September 12–19, 1999*, Springer, 2001, 196–211. https://doi.org/10.1007/978-3-642-59448-9_13

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