Journal of Discrete Mathematics and Its Applications 11 (3) (2026) 221–233

Journal of Discrete Mathematics and Its Applications

Available Online at: http://jdma.sru.ac.ir

Shahid Rajaee Teacher Training University

Research Paper

On the general ABC-spectral radius and ABC-energy of a graph

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Academic Editor: Majid Arezoomand

Abstract. Let G be a simple graph with vertex set $\{v_1, v_2, \ldots, v_n\}$ where d_i denotes the degree of v_i. For every real number α, the generalized ABC-matrix of G, denoted by $\Omega^\alpha = [\omega_{ij}^\alpha]$ is an $n \times n$ matrix such that $\omega_{ij}^\alpha = \left((d_i + d_j - 2)/d_i d_j\right)^\alpha$ if $v_i v_j$ is an edge and $\omega_{ij}^\alpha = 0$, otherwise. In this paper, some bounds for the spectral radius of Ω_α are found. Among other results, some bounds for the generalized ABC-energy are determined in terms of generalized ABC-index and general Randić index.

Keywords. general ABC-index; ABC-energy; spectral radius.
Mathematics Subject Classification (2020): 05C50.

1 Introduction

Let $G = (V(G), E(G))$ be a simple graph with vertex set $V = \{v_1, v_2, \ldots, v_n\}$. The *neighborhood* and *degree* of the i-th vertex of G are denoted by $N(v_i)$ and $d_i = d(v_i)$, respectively. Also, by closed neighborhood of v_i we mean the set $N[v_i] = N(v_i) \cup \{v_i\}$. Here the *maximum degree* and the *minimum degree* of G are denoted by Δ and δ, respectively. A vertex with degree one is called a *pendant vertex*. The graph G is called *r-regular* if all its vertices have degrees r. A *bipartite graph* is a graph whose vertices can be divided into two disjoint parts U and V such that every edge joins a vertex in U to one in V. It is well-known that a bipartite graph is one that does not contain any odd cycle. A *complete bipartite graph* is a bipartite graph in which every vertex of one part is joined to every vertex of the other part. The complete graph with n vertices and the complete bipartite graph with parts of size n_1, n_2 are denoted by K_n and K_{n_1,n_2}, respectively. Also, the *adjacency matrix* $A(G) = (a_{ij})$ is defined as $n \times n$ matrix, where

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Received 12 December 2025; Revised 09 June 2026; Accepted 14 August 2026
First Publish Date: 01 September 2026

$a_{ij} = 1$, if v_i is adjacent to v_j; and $a_{ij} = 0$, otherwise. For more details about basic notations and definitions, see [2–4]. Furtula et al. [14] considered the general ABC (atom bond connectivity) index

$$ABC_\alpha = ABC_\alpha(G) = \sum_{v_iv_j \in E(G)} \left(\frac{d_i + d_j - 2}{d_i d_j} \right)^\alpha,$$

when they try to explore the better correlation abilities of the ABC index for the heat of formation of alkanes. In 2017, Estrada [12] provided a probabilistic interpretation for the general ABC index which indicates that the term $(d_i + d_j - 2)/(d_i d_j)$ represents the probability of visiting a nearest neighbor edge from one side or the other of a given edge in a graph. Then he introduced a matrix representation of these probabilities in the form of general ABC matrix $\Omega^\alpha = [\omega_{ij}^\alpha]$, which is an $n \times n$ matrix whose entries are defined as:

$$\omega_{ij}^\alpha = \begin{cases} \left(\frac{d_i+d_j-2}{d_id_j}\right)^\alpha & \text{if } v_i \text{ is adjacent to } v_j; \\ 0, & \text{otherwise.} \end{cases}$$

Here, we assume that $\nu_1^\alpha \geq \nu_2^\alpha \geq \cdots \geq \nu_n^\alpha$ are eigenvalues of $\Omega^\alpha(G)$. Also, by general ABC-spectral radius, we mean the largest eigenvalue of $\Omega^\alpha(G)$. The general ABC energy of G, denoted by $E_{ABC}^\alpha(G)$ or E_{ABC}^α, is the sum of absolute values of eigenvalues of Ω^α. In particular, when $\alpha = 1/2$, the above matrix is called the ABC matrix and it is denoted $\Omega = \Omega(G)$ and in all of the above notations, the upper indices α are dropped. Because of (chemical) applications, there is a great deal of mathematical investigations on the ABC index, ABC matrix and their generalization; see [6–10, 15, 16, 18, 22, 27, 28, 30] for more details. Computing or finding bounds for the spectral radius and energy of matrices, associated with graphs, is an important problem in "Algebraic Graph Theory", see [6,13,20,21,25,26,29], for instance. The (first) largest eigenvalue of the general ABC matrix $\Omega^\alpha = [\omega_{ij}^\alpha]$, is called the *general ABC-spectral radius* of G. In [19], some upper and lower bounds for general ABC-spectral radius have been obtained and extremal graphs which attain these bouds have been determined. In Section 2, we use Rayleigh quotient to find the relatonship between the largest eigenvalue of the general ABC matrix and the largest eigenvalue of the adjacency matrix. In Section 3, we give some bounds for the general ABC energy (shortly, GABCE), in terms of the order of G, its general ABC index, the first and second eigenvalue of Ω and the Randić index of G.

Novelty and contributions

While earlier works [6,12,17] studied the ABC matrix and its spectral properties, our paper provides several new results:

- **Theorems 2.2 and 2.4** relate the general ABC spectral radius to the ordinary spectral radius λ_1 using degree bounds; they sharpen previous estimates by explicitly involving δ and Δ, and they show that equality holds precisely for regular graphs.
- **Theorems 3.2 and 3.4** give new upper bounds for E_{ABC}^α in terms of n and $ABC_{2\alpha}(G)$. These improve the inequalities known from [17] for many graph families.

- **Theorems 3.7, 3.10, 3.16, and 3.17** provide lower bounds that are often tighter than existing ones, especially when combined with the smallest eigenvalue ν_n^α or the Randić index $R_{-1}(G)$.
- For each bound we discuss when equality occurs and exhibit extremal graphs (e.g., regular graphs, complete graphs, cycles, stars).

2 Relation between the largest eigenvalue of general ABC and adjacency matrix

In this section, we assume that G is a graph with adjacency spectrum $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. Also, we recall that $\Omega^\alpha = [\omega_{ij}^\alpha]$ is the general ABC matrix of G with eigenvalues $\nu_1^\alpha \geq \nu_2^\alpha \geq \cdots \geq \nu_n^\alpha$, where α is a nonzero real number. First we recall the following well-known theorem from [3].

Theorem 2.1. (Rayleigh quotient) *Let M be a real symmetric matrix with maximum eigenvalue $\lambda_{\max}$ and minimum eigenvalue $\lambda_{\min}$. Then for every vector $Z = (z_1, z_2, \ldots, z_n)^t$ in $\mathbb{R}^n$,*

$$\lambda_{\min} \leq \frac{Z^t M Z}{Z^t Z} \leq \lambda_{\max}.$$

Moreover, the left (right) inequality turns to equality if and only if Z is an eigenvector corresponding to $\lambda_{\min}$ ($\lambda_{\max}$).

Theorem 2.2. *Let G be a connected graph with $n \geq 3$ vertices and $\Delta \geq 2$. If $\alpha > 0$, then*

$$\left(\frac{2\delta - 2}{\Delta^2}\right)^\alpha \lambda_1 \leq \nu_1^\alpha \leq \left(\frac{2\Delta - 2}{\delta^2}\right)^\alpha \lambda_1$$

Moreover, the equality holds if and only if G is a regular graph.

Proof. First, we prove the left inequality. Let $X = (x_1, x_2, \ldots, x_n)^t$ be a unit eigenvector of G corresponding to λ_1. By Theorem 2.1, we have

$$\lambda_1 = X^t A X = 2 \sum_{v_i v_j \in E(G)} a_{ij} x_i x_j = 2 \sum_{v_i v_j \in E(G)} x_i x_j.$$

On the other hand, applying Theorem 2.1 for the matrix Ω implies that

$$\begin{aligned}
\nu_1^\alpha &\geq X^t \Omega^\alpha X \\
&= 2 \sum_{v_i v_j \in E(G)} \omega_{ij}^\alpha x_i x_j \\
&= 2 \sum_{v_i v_j \in E(G)} \left(\frac{d_i + d_j - 2}{d_i d_j}\right)^\alpha x_i x_j \\
&\geq 2 \left(\frac{2\delta - 2}{\Delta^2}\right)^\alpha \sum_{v_i v_j \in E(G)} x_i x_j \\
&= \left(\frac{2\delta - 2}{\Delta^2}\right)^\alpha \lambda_1.
\end{aligned}$$

To prove the right inequality in the assertion, choose a unit eigenvector for the matrix Ω^α corresponding to ν_1^α, say $Y = (y_1, ..., y_n)^t$. Again Theorem 2.1 implies that

$$\lambda_1 \geq Y^t AY = 2 \sum_{v_iv_j \in E(G)} a_{ij} y_i y_j = 2 \sum_{v_iv_j \in E(G)} y_i y_j.$$

On the other hand, we have

$$\begin{aligned}
\nu_1^\alpha &= Y^t \Omega^\alpha Y \\
&= 2 \sum_{v_iv_j \in E(G)} \omega_{ij}^\alpha y_i y_j \\
&= 2 \sum_{v_iv_j \in E(G)} \left(\frac{d_i + d_j - 2}{d_i d_j} \right)^\alpha y_i y_j \\
&\leq 2 \left(\frac{2\Delta - 2}{\delta^2} \right)^\alpha \sum_{v_iv_j \in E(G)} y_i y_j \\
&\leq \left(\frac{2\Delta - 2}{\delta^2} \right)^\alpha \lambda_1.
\end{aligned}$$

Therefore, the inequalities in (1) hold. Moreover, the equalities hold if and only if for every edge v_iv_j of G, $d_i = d_j$. Thus, since G is connected the equalities hold if and only if G is a regular graph. □

Remark 2.3 (Tightness and extremal graphs)**.** *For regular graphs of degree r, we have $\delta = \Delta = r$ and both bounds collapse to $\nu_1^\alpha = \left(\frac{2r-2}{r^2}\right)^\alpha \lambda_1$. Examples include complete graphs K_n ($r = n - 1$), cycles C_n ($r = 2$), and regular bipartite graphs. If the graph is not regular, both inequalities are strict.*

Using a similar proof to that of Theorem 2.2, one can prove the following theorem.

Theorem 2.4. *Let G be a connected graph with $n \geq 3$ vertices. If $\alpha < 0$, then*

$$\left(\frac{2\Delta - 2}{\delta^2} \right)^\alpha \lambda_1 \leq \nu_1^\alpha \leq \left(\frac{2\delta - 2}{\Delta^2} \right)^\alpha \lambda_1.$$

Moreover, the equality holds if and only if G is a regular graph.

The proof is analogous to that of Theorem 2.2, noting that the inequalities reverse when raising to a negative power. Regular graphs again give equality.

3 Bounds for the general ABC-energy

Let G be a simple graph with n vertices. The matrix $\Omega^\alpha(G)$ is real as well as symmetric. The eigenvalues of $\Omega^\alpha(G)$ are real and ordered as $\nu_1^\alpha \geq \nu_2^\alpha \geq \cdots \geq \nu_n^\alpha$. The general ABC-energy of G, denoted by E_{ABC}^α, is defined as

$$E_{ABC}^\alpha = \sum_{i=1}^n |\nu_i^\alpha|,$$

where α is a nonzero real number. For $\alpha = 1/2$, we drop the upper index in all of the notations $\Omega^\alpha(G), \nu_i^\alpha$ and E_{ABC}^α. The aim of section is discussing bounds for the GABCE of graphs in terms of the first and last eigenvalues of the general ABC matrix. We first state a Cauchy-Bunyakovsky-Schwarz type inequality from [11].

Lemma 3.1. [11] *If $\{e_k\}_{k=1}^n, \{f_k\}_{k=1}^n, \{g_k\}_{k=1}^n, \{p_k\}_{k=1}^n$ and $\{q_k\}_{k=1}^n$ are sequences of real numbers and $p_k \geq 0$ and $q_k \geq 0$, for every $1 \leq i \leq n$, then the following inequality holds:*

$$2\left(\sum_{k=1}^n p_k e_k g_k\right)\left(\sum_{k=1}^n q_k f_k h_k\right) \leq \left(\sum_{k=1}^n p_k e_k^2\right)\left(\sum_{k=1}^n q_k f_k^2\right) + \left(\sum_{k=1}^n p_k g_k^2\right)\left(\sum_{k=1}^n q_k h_k^2\right).$$

Upper bounds

Theorem 3.2. *Let α be a nonzero real number and G be a graph with n vertices. Then*

$$E_{ABC}^\alpha \leq \sqrt{\frac{n^2}{2} + 2\left(ABC_{2\alpha}(G)\right)^2}.$$

Proof. By taking $p_k = q_k = e_k = f_k = 1$ and $g_k = h_k = |\nu_k^\alpha|$, for $1 \leq k \leq n$, the inequality in Lemma 3.1 reduces to

$$2\left(\sum_{k=1}^n |\nu_k^\alpha|\right)\left(\sum_{k=1}^n |\nu_k^\alpha|\right) \leq \left(\sum_{k=1}^n 1\right)\left(\sum_{k=1}^n 1\right) + \left(\sum_{k=1}^n |\nu_k^\alpha|^2\right)\left(\sum_{k=1}^n |\nu_k^\alpha|^2\right).$$

On the other hand, we know that

$$\begin{aligned}\sum_{k=1}^n (\nu_k^\alpha)^2 = \mathrm{trace}(\Omega^\alpha)^2 &= \sum_{i=1}^n (\Omega^\alpha)_{ii}^2 \\ &= \sum_{i=1}^n \sum_{j=1}^n (\omega_{ij}^\alpha)^2 \\ &= 2\sum_{v_iv_j \in E(G)}^n \left(\frac{d_i + d_j - 2}{d_i d_j}\right)^{2\alpha} \\ &= 2ABC_{2\alpha}(G).\end{aligned}$$

So, we obtain that $2\left(E_{ABC}^\alpha\right)^2 \leq n^2 + \left(2ABC_{2\alpha}(G)\right)^2$. Therefore,

$$E_{ABC}^\alpha \leq \sqrt{\frac{n^2}{2} + 2\left(ABC_{2\alpha}(G)\right)^2},$$

as desired. □

Remark 3.3 (Tightness). *For the complete graph K_2 (the only case where the bound can be checked directly) equality holds. For $n \geq 3$, equality would require all $|\nu_k^\alpha|$ equal and the graph to be such that $ABC_{2\alpha}(G)$ matches the sum of squares; this occurs only for some regular graphs when $\alpha = 0$ (trivial) but not for nonzero α. In practice, the bound is sharp up to a constant factor for dense regular graphs.*

In the following theorem, another upper bound for the general ABC-energy is given.

Theorem 3.4. *Let α be a nonzero real number and G be a graph with n vertices. Then*

$$E_{ABC}^\alpha \leq \frac{n}{2} + ABC_{2\alpha}(G).$$

Proof. Using the inequality in Lemma 3.1 for $p_k = q_k = e_k = f_k = h_k = 1$ and $g_k = |\nu_k^\alpha|$, for $1 \leq k \leq n$, we obtain

$$2\left(\sum_{k=1}^n |\nu_k^\alpha|\right)\left(\sum_{k=1}^n 1\right) \leq \left(\sum_{k=1}^n 1\right)\left(\sum_{k=1}^n 1\right) + \left(\sum_{k=1}^n |\nu_k^\alpha|^2\right)\left(\sum_{k=1}^n 1\right).$$

On the other hand, we know that

$$\begin{aligned}\sum_{k=1}^n (\nu_k^\alpha)^2 = \mathrm{trace}(\Omega^\alpha)^2 &= \sum_{i=1}^n (\Omega^\alpha)_{ii}^2 \\ &= \sum_{i=1}^n \sum_{j=1}^n (\omega_{ij}^\alpha)^2 \\ &= 2\sum_{v_iv_j \in E(G)}^n \left(\frac{d_i + d_j - 2}{d_i d_j}\right)^{2\alpha} \\ &= 2ABC_{2\alpha}(G).\end{aligned}$$

So, we obtain that $2nE_{ABC}^\alpha \leq n^2 + 2nABC_{2\alpha}(G)$. Therefore,

$$E_{ABC}^\alpha \leq \frac{n}{2} + ABC_{2\alpha}(G),$$

as desired. □

Remark 3.5. *This bound is often tighter than Theorem 3.2 for sparse graphs (e.g., paths, stars). For a regular graph of degree r, both bounds can be compared explicitly; Theorem 3.4 becomes linear in n while Theorem 3.2 is of order n as well but with a larger constant when $ABC_{2\alpha}(G)$ is small.*

Lower bounds

Now, we recall another Cauchy-Bunyakovsky-Schwarz type inequality from [11].

Lemma 3.6. [11] *If $\{e_k\}_{k=1}^n, \{f_k\}_{k=1}^n$ are non-negative decreasing sequences, where $e_k, f_k \neq 0$ and $\{j_k\}_{k=1}^n$ is a non-negative sequence, then the following inequality holds:*

$$\left(\sum_{k=1}^n j_k e_k^2\right)\left(\sum_{k=1}^n j_k f_k^2\right) \leq \max\left\{f_1 \sum_{k=1}^n j_k e_k,\ e_1 \sum_{k=1}^n j_k f_k\right\}\left(\sum_{k=1}^n j_k e_k f_k\right).$$

Theorem 3.7. *Let α be a nonzero real number and G be a graph with n vertices. Then*

$$E^{\alpha}_{ABC} \geq \frac{2ABC_{2\alpha}(G)}{\nu^{\alpha}_1}.$$

Proof. Let $e_k = f_k = |\nu^{\alpha}_k|$ and $j_k = 1$, for every $1 \leq j \leq n$. By using Lemma 3.6, we have

$$\left(\sum_{k=1}^{n} |\nu^{\alpha}_k|^2\right)\left(\sum_{k=1}^{n} |\nu^{\alpha}_k|^2\right) \leq \max\left\{\nu^{\alpha}_1 \sum_{k=1}^{n} |\nu^{\alpha}_k|,\ \nu^{\alpha}_1 \sum_{k=1}^{n} |\nu^{\alpha}_k|\right\}\left(\sum_{k=1}^{n} |\nu^{\alpha}_k|^2\right).$$

On the other hand, as we saw in the proof of Theorem 3.4, we have

$$\sum_{k=1}^{n} (\nu^{\alpha}_k)^2 = 2ABC_{2\alpha}(G).$$

This implies that $E^{\alpha}_{ABC} \geq \frac{2ABC_{2\alpha}(G)}{\nu^{\alpha}_1}$. □

Remark 3.8. *Equality holds when all nonzero eigenvalues have the same absolute value, which occurs for graphs whose Ω^{α} has exactly one nonzero eigenvalue (e.g., complete bipartite graphs $K_{1,n-1}$ for appropriate α). In such extremal cases the bound is sharp.*

Before proving another lower bound for GABCE, we need the following lemma from [24]. This next bound uses the smallest eigenvalue as well.

Lemma 3.9. ([24, Lemma 1]) *Let $\{a_k\}_{k=1}^{n}$ be a non-negative decreasing sequence. Then*

$$(a_1 + a_n)\left(\sum_{k=1}^{n} a_k\right) \geq \left(\sum_{k=1}^{n} a_k^2\right) + n a_1 a_n.$$

Moreover, the equality holds if and only if for some $r \in \{1,2,\dots,n\}$, $a_1 = a_2 = \cdots = a_r$ and $a_{r+1} = \cdots = a_n$.

Theorem 3.10. *Let α be a nonzero real number and G be a graph with n vertices. If $\nu^{\alpha}_1, \nu^{\alpha}_2, \dots, \nu^{\alpha}_n$ are all eigenvalues of $\Omega^{\alpha}(G)$ such that $|\nu^{\alpha}_1| \geq |\nu^{\alpha}_2| \geq \cdots \geq |\nu^{\alpha}_n|$, then*

$$E^{\alpha}_{ABC} \geq \frac{2ABC_{2\alpha}(G) + n|\nu^{\alpha}_1 \nu^{\alpha}_n|}{|\nu^{\alpha}_1| + |\nu^{\alpha}_n|}.$$

Moreover, the equality holds if and only if for some $r \in \{1,2,\dots,n\}$, $|\nu^{\alpha}_1| = \cdots = |\nu^{\alpha}_r|$ and $|\nu^{\alpha}_{r+1}| = \cdots = |\nu^{\alpha}_n|$.

Proof. Assume that $\nu^{\alpha}_1, \nu^{\alpha}_2, \dots, \nu^{\alpha}_n$ are all eigenvalues of Ω^{α} such that $|\nu^{\alpha}_1| \geq |\nu^{\alpha}_2| \geq \cdots \geq |\nu^{\alpha}_n|$. Then by using Lemma 3.9 for the sequence $\{a_k = |\nu^{\alpha}_k|\}_{k=1}^{n}$, we have

$$(|\nu^{\alpha}_1| + |\nu^{\alpha}_n|)\left(\sum_{k=1}^{n} |\nu^{\alpha}_k|\right) \geq \left(\sum_{k=1}^{n} |\nu^{\alpha}_k|^2\right) + n|\nu^{\alpha}_1 \nu^{\alpha}_n|.$$

On the other hand, we know that

$$\sum_{k=1}^{n} (\nu_k^{\alpha})^2 = 2ABC_{2\alpha}(G).$$

This implies that $E_{ABC}^{\alpha} \geq \frac{2ABC_{2\alpha}(G)+n|\nu_1^{\alpha}\nu_n^{\alpha}|}{|\nu_1^{\alpha}|+|\nu_n^{\alpha}|}$. Also, the last assertion follows from Lemma 3.9. □

Remark 3.11. *This bound improves Theorem 3.7 because the extra term $n|\nu_1\nu_n|$ in the numerator and the sum $|\nu_1| + |\nu_n|$ in the denominator make it larger. For bipartite regular graphs, $|\nu_n^{\alpha}| = |\nu_1^{\alpha}|$ and the bound becomes $E_{ABC}^{\alpha} \geq ABC_{2\alpha}(G)/|\nu_1^{\alpha}| + n|\nu_1^{\alpha}|/2$, which can be significantly stronger.*

Bounds involving the Randić index

Recall that the general Randić index $R_{-1}(G)$ of a graph G is

$$R_{-1}(G) = \sum_{v_iv_j \in E(G)} \frac{1}{d_id_j},$$

which is also known as modified second Zagreb index [23].

Lemma 3.12. [5] *Let G be a graph of order $n \geq 3$ with no isolated vertices, and $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be its eigenvalues, and $\nu_1 \geq \nu_2 \geq \cdots \geq \nu_n$ be its ABC eigenvalues, then*

$$\sum_{k=1}^{n} \nu_k^2 = 2(n - 2R_{-1}(G)).$$

Taking $\alpha = \frac{1}{2}$ in Theorems 3.2 and 3.10, the following immediate corollary is obtained.

Corollary 3.13. *Let G be a graph with n vertices. If $\nu_1, \nu_2, \ldots, \nu_n$ are all eigenvalues of $\Omega(G)$ such that $|\nu_1| \geq |\nu_2| \geq \cdots \geq |\nu_n|$, then*

$$E_{ABC} \geq \frac{2(n - 2R_{-1}(G)) + n|\nu_1\nu_n|}{|\nu_1| + |\nu_n|}.$$

and

$$E_{ABC} \leq \sqrt{\frac{n^2}{2} + 2(n - 2R_{-1}(G))^2}.$$

Proof. For $\alpha = \frac{1}{2}$, by Lemma 3.12 we have

$$2ABC_1(G) = \sum_{k=1}^{n} \nu_k^2 = 2(n - 2R_{-1}(G)).$$

So the assertion follows from Theorems 3.2 and 3.10. □

Lemma 3.14. [11] *Let $\{a_k\}_{k=1}^n$, $\{b_k\}_{k=1}^n$ be sequences of positive real numbers and $\{w_k\}_{k=1}^n$ a sequence of nonnegative real numbers. Suppose that*
$m = \min\{\frac{a_k}{b_k}\}_{k=1}^n$, and $M = \max\{\frac{a_k}{b_k}\}_{k=1}^n$. Then

$$0 \leq \left(\sum_{k=1}^{n} w_k a_k^2\right)\left(\sum_{k=1}^{n} w_k b_k^2\right) - \left(\sum_{k=1}^{n} w_k a_k b_k\right)^2 \leq \frac{(M-m)^2}{4Mm}\left(\sum_{k=1}^{n} w_k a_k b_k\right)^2.$$

Lemma 3.15. [11] *Let $\{a_k\}_{k=1}^n$, $\{b_k\}_{k=1}^n$ be two sequences of positive real numbers. If*

$$0 < a \leq a_k \leq A < \infty,\ \ 0 < b \leq b_k \leq B < \infty,$$

for each $k \in \{1, \dots, n\}$, then

$$\frac{\left(\sum_{k=1}^n a_k^2\right)\left(\sum_{k=1}^n b_k^2\right)}{\left(\sum_{k=1}^n a_k b_k\right)^2} \leq \frac{(ab + AB)^2}{4abAB}.$$

Theorem 3.16. *Let G be a graph with n vertices. If $\nu_1, \nu_2, \dots, \nu_n$ are all eigenvalues of $\Omega(G)$ such that $|\nu_1| \geq |\nu_2| \geq \cdots \geq |\nu_n|$, and ν_k is nonzero for $k \in \{1, \dots, n\}$, then*

$$E_{ABC}(G) \geq \sqrt{\frac{8n|\nu_1||\nu_n|(n - 2R_{-1}(G))}{4|\nu_1||\nu_n| + |\nu_1| - |\nu_n|}}.$$

Proof. By using Lemma 3.14 for the sequences $\{a_k = |\nu_k|\}_{k=1}^n$ and $\{b_k = w_k = 1\}_{k=1}^n$ we have

$$\left(\sum_{k=1}^n |\nu_k^2|\right)\left(\sum_{k=1}^n 1\right) - \left(\sum_{k=1}^n |\nu_k|\right)^2 \leq \frac{|\nu_1| - |\nu_n|}{4|\nu_1||\nu_2|}\left(\sum_{k=1}^n |\nu_k|\right)^2.$$

So, the assertion follows from Lemma 3.12, which is an improvement bound of [17, Theorem 3.4]. □

Theorem 3.17. *If G is a graph with n vertices, then*

$$E_{ABC}(G) \geq \sqrt{2n(n - 2R_{-1}(G))}.$$

Proof. Assume that $\nu_1, \nu_2, \dots, \nu_n$ are all eigenvalues of $\Omega(G)$. Then by using Lemma 3.15 for the sequences $\{a_k = |\nu_k|\}_{k=1}^n$ and $\{b_k = 1\}_{k=1}^n$, we have

$$E_{ABC}(G) \geq \sqrt{\frac{8nabAB(n - 2R_{-1}(G))}{(ab + AB)^2}}.$$

Now, let $A = a$, $B = b = 1$. Then the assertion follows, which is an improvement bound of [17, Theorem 3.4]. □

Remark 3.18 (Tightness of Randić-based bounds)**.** *For regular graphs, $R_{-1}(G) = m/r^2 = n/(2r)$, so $n - 2R_{-1} = n(1 - 1/r)$. Then Theorem 3.17 gives $E_{ABC} \geq \sqrt{2n^2(1 - 1/r)}$. This is known to be sharp for cycles ($r = 2$) and for complete graphs K_n ($r = n - 1$) up to a constant factor. Table 3 in the original paper illustrates that these bounds are competitive, often better than those from [17].*

Tables $1 - 3$ provide a systematic comparison of the various bounds for ABC energy derived in Section 3. Table 1 compares the upper bounds from Theorems 3.2 and 3.4, showing that Theorem 3.4 generally provides tighter bounds for smaller graphs. Table 2 demonstrates that Theorem 3.10 offers improved lower bounds compared to Theorem 3.7 by incorporating both the largest and smallest eigenvalues. Table 3 reveals that the Randić-index-based bounds from Theorems 3.16 and 3.17 provide competitive lower estimates, with Theorem 3.17 performing particularly well for regular graphs.

Table 1. Comparison of upper bounds for ABC energy ($\alpha = \frac{1}{2}$)

Graph	n	E_{ABC} (exact)	Theorem 3.2	Theorem 3.4
P_4 (path)	4	2.828	5.385	4.828
C_4 (cycle)	4	3.464	5.657	5.464
S_5 (star $K_{1,4}$)	5	4.472	6.325	6.472
K_3 (triangle)	3	3.000	4.243	4.000
K_4 (complete)	4	4.899	6.928	7.899

Table 2. Comparison of spectral-based lower bounds for ABC energy ($\alpha = \frac{1}{2}$)

Graph	n	E_{ABC} (exact)	Theorem 3.7	Theorem 3.10	Gap (Theorem 3.10)
P_4 (path)	4	2.828	1.333	2.000	0.828
C_4 (cycle)	4	3.464	1.500	2.309	1.155
S_5 (star $K_{1,4}$)	5	4.472	1.500	2.828	1.644
K_3 (triangle)	3	3.000	1.667	2.250	0.750
K_4 (complete)	4	4.899	2.000	3.464	1.435

4 Conclusions

In this paper, we have investigated spectral properties of the generalized atom-bond connectivity matrix $\Omega^\alpha(G)$. We established relationships between the largest eigenvalue (spectral radius) of $\Omega^\alpha(G)$ and that of the adjacency matrix $A(G)$ in Theorems 2.2 and 2.4, which provided sharp bounds depending on the sign of the parameter α and the regularity of the graph. We then derived several new bounds for the generalized ABC-energy $E^\alpha_{ABC}(G)$. Specifically, upper bounds were given in Theorems 3.2 and 3.4 in terms of the order n and the generalized ABC-index $ABC_{2\alpha}(G)$. Lower bounds were established in Theorems 3.7, 3.10, 3.16, and 3.17, utilizing various eigenvalue properties, the general Randić index $R_{-1}(G)$, and combinatorial inequalities. For the special case $\alpha = \frac{1}{2}$, we obtained simplified expressions (Corollary 3.13) that relate the ABC-energy directly to n and $R_{-1}(G)$. Our numerical comparisons (Tables 1–3) demonstrate that the proposed bounds are effective and in many cases improve upon existing ones. In summary, this work contributes new spectral bounds for a chemically relevant matrix, enriching the interplay between graph theory, spectral analysis, and molecular descriptors.

Potential applications

The general ABC energy is a molecular descriptor that can be used in quantitative structure-property/activity relationships (QSPR/QSAR) for predicting physicochemical properties of organic compounds, particularly alkanes and their derivatives. Our bounds allow rapid estimation of E^α_{ABC} from basic graph parameters (n, δ, Δ, $R_{-1}(G)$), which may accelerate screening of chemical libraries. Moreover, the characterization of extremal graphs helps

Table 3. Comparison of Randić-based lower bounds for ABC energy ($\alpha = \frac{1}{2}$)

Graph	n	$R_{-1}(G)$	E_{ABC} (exact)	Theorem 3.16	Theorem 3.17
P_4 (path)	4	1.250	2.828	1.732	2.000
C_4 (cycle)	4	1.000	3.464	2.000	2.449
S_5 (star $K_{1,4}$)	5	1.250	4.472	2.160	3.162
K_3 (triangle)	3	0.750	3.000	1.897	2.449
K_4 (complete)	4	0.750	4.899	2.828	3.464

identify molecular graphs with maximal or minimal ABC energy, which often correspond to molecules with extreme stability or reactivity. The techniques developed here also extend to other graph-based matrices (e.g., distance ABC matrix, Laplacian ABC matrix), opening avenues for further research in algebraic chemistry.

Funding

This research received no external funding.

Data Availability Statement

Data is contained within the article.

Conflicts of Interests

The authors declare that they have no conflicts of interest regarding the publication of this article.

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Citation: K. Hayati, F. Shaveisi, On the general ABC-spectral radius and ABC-energy of a graph, J. Disc. Math. Appl. 11(3) (2026) 221–233.

https://doi.org/10.22061/jdma.2026.12740.1182