

The *ABC* Spectrum of Caterpillars and Applications

Enide Andrade^a, Eber Lenes^b, María Robbiano^{c,*},
Bernardo San Martín^d

^a CIDMA-Center for Research and Development in Mathematics and Applications, Department of Mathematics, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal

^b Área de Ciencias Básicas Exactas, Grupo de Investigación Deartica, Universidad del Sinú, Cartagena, Colombia

^{c,d} Departamento de Matemáticas, Universidad Católica del Norte, Avenida Angamos, Antofagasta, 0610, Chile

enide@ua.pt, eber.lenes@unisinu.edu.co, mrobbiano@ucn.cl,

sanmarti@ucn.cl

(Received March 18, 2026)

Abstract

Let G be an undirected simple graph with n vertices and let d_i be the degree of the vertex i in G . The *ABC* matrix of G is a square matrix of order n whose (i, j) - entry is $\sqrt{\frac{d_i + d_j - 2}{d_i d_j}}$, if the vertices v_i and v_j are connected and zero otherwise. Let H be a simple undirected graph with r vertices, $v_1, v_2, \dots, v_r$ and $G_1, G_2, \dots, G_r$, r disjoint p_j - regular graphs, $j = 1, \dots, r$. The H -join of $G_1, G_2, \dots, G_r$, denoted by $H[G_1, G_2, \dots, G_r]$, is the graph G obtained by joining each vertex of G_i to all vertices of G_j whenever the vertices v_i and v_j are neighbors in H for all $1 \leq i, j \leq r$. In this work, the *ABC* spectrum, the *ABC* spectral radius, and the *ABC* energy of certain caterpillars trees are studied.

*Corresponding author.

1 Introduction

Let G be a graph with vertex set $\mathcal{V}(G)$ and edge set $\mathcal{E}(G)$. A vertex $v_i \in \mathcal{V}(G)$ and an edge $v_i v_j \in \mathcal{E}(G)$, is sometimes just denoted by i and ij , respectively. It is known that the cardinality of $\mathcal{V}(G)$ is the *order* of G . A path of order r , P_r , is a graph G with r distinct vertices, $v_1, v_2, \dots, v_r$ such that $\mathcal{E}(G) = \{v_i v_{i+1} : i = 1, \dots, r-1\}$. If $uv \in \mathcal{E}(G)$ we say that u and v are connected (or linked) or that u and v are neighbors. A *pendant vertex* or *leaf* is a vertex that has only one neighbor. A tree is a graph where any two vertices are connected by exactly one path. A rooted tree is a tree in which a special vertex is singled out. This vertex is called the *root* of the tree. For $r \geq 1$, a *star* with $r+1$ vertices, S_{r+1} , is a tree that has a rooted vertex, v , and r neighbors of v that are pendant vertices.

A *caterpillar* tree (also known as Gutman tree or benzenoid tree) is a tree of order $n \geq 4$ such that, when all its pendant vertices are removed the resulting structure is a path with at least two vertices. Let $r \geq 2$. The caterpillar tree $T(q_1, \dots, q_r)$ is then constructed by identifying the central vertex of each star S_{q_i+1} with the i -th vertex of the path P_r , $i = 1, \dots, r$. Then, the order of $T(q_1, \dots, q_r)$ is

$$n = r + \sum_{i=1}^r q_i.$$

Caterpillar trees are very important in Chemistry. Check for instance [16], where the author shows that certain benzenoid systems (models of aromatic hydrocarbons) can be analysed via graph structures closely related to caterpillars. In this setting, the sextet polynomial, which encodes the number of aromatic sextets and thus reflects molecular stability, can be connected to characteristic polynomials of these graphs. This illustrates how caterpillar-like structures naturally arise in Chemical Graph Theory and help capture chemically relevant properties such as electron delocalization.

Further notation will be introduced as necessary throughout the text. The set of neighbors of $i \in \mathcal{V}(G)$ is denoted by $N_G(i)$ and the *degree* of i , which is the cardinality of this set, is denoted by d_i .

A vertex of degree 0 is called an *isolated* vertex. If $d_i = k$, for all $i \in \mathcal{V}(G)$ we say that G is a k -regular graph. The largest and smallest degree of the vertices of G are denoted by $\Delta(G)$ (or simply, Δ) and $\delta(G)$, (or, simply δ), respectively. A graph is called (Δ, δ) -*bipartite semiregular* if it is bipartite and each vertex in the first (respectively, second) set of the bipartition has degree $\Delta(G)$ (respectively, $\delta(G)$). A k -regular simple graph G on ν vertices is *strongly k -regular* if there exist positive integers k , λ , and μ such that every vertex has k neighbors, every adjacent pair of vertices has λ common neighbors, and every nonadjacent pair of vertices has μ common neighbors [19]. A strongly regular graph is denoted by $\text{sgr}(\nu, k, \lambda, \mu)$.

The adjacency matrix of G is denoted by $A_G = (a_{ij})_{1 \leq i, j \leq n}$, where

$$a_{ij} = \begin{cases} 1 & ij \in \mathcal{E}(G) \\ 0 & \text{otherwise.} \end{cases}$$

The Randić matrix $R = (r_{ij})_{1 \leq i, j \leq n}$ is defined by $r_{ij} = \frac{1}{\sqrt{d_i d_j}}$, if the i -th and j -th vertices are neighbors and $r_{ij} = 0$, otherwise. The Randić energy is the sum of the absolute values of eigenvalues of R . The general Randić index or branching index was defined in [20] as

$$R_{-1}(G) = \sum_{ij \in \mathcal{E}(G)} \frac{1}{d_i d_j} \quad (1)$$

Among other results, in [21] it is shown that

$$\frac{n}{2\Delta(G)} \leq R_{-1}(G) \leq \frac{n}{2\delta(G)}, \quad (2)$$

where the equality holds if and only if G is a regular graph. For a square matrix M , the set of its eigenvalues, is denoted by σ_M . If the eigenvalues of M are ordered in non increasing order, we denote by $\lambda_i(M)$ its i -th eigenvalue, for $i = 1, \dots, n$. The multiplicity m of an eigenvalue α of M is indicated by $\alpha^{[m]}$. Thus, the set of eigenvalues of M is

$$\sigma_M = \left\{ \alpha_1^{[m_1]}, \dots, \alpha_s^{[m_s]} \right\}.$$

If $M = A_G$ the set σ_M is denoted by σ_G and it is called the *spectrum* of the graph G . If G has n vertices, the elements of σ_G are ordered as $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$.

If α is an eigenvalue of a square matrix M and $\mathbf{x}$ is one of its eigenvectors, the pair $(\alpha, \mathbf{x})$ is an *eigenpair* of M . If M is a square matrix, its *spectral radius* is given by

$$\rho(M) = \max\{|\lambda| : \lambda \in \sigma_M\}.$$

It is well known that the largest eigenvalue of a non-negative matrix (a matrix whose entries are all non-negative) and its spectral radius coincide, [18]. Moreover, the nonnegative eigenvector of a non-negative matrix is called *maximal eigenvector*.

Notation: K_p denotes the complete graph with p vertices. The graph complement of G is $\overline{G}$. The graph $\overline{K}_n$ is the empty graph with n vertices. The join of the graphs G and H is denoted by $G \vee H$.

A complete multipartite graph with partitions of size $|V_1| = n_1, |V_2| = n_2, \dots, |V_p| = n_p$, is denoted by $K_{n_1, n_2, \dots, n_p}$. We denote by $G \cup H$ the vertex-disjoint union of the graphs G and H . In particular, kG is the vertex-disjoint union of k copies of the graph G . The null square matrix of arbitrary order will be denoted by $\mathbf{O}$. The all ones vector and the identity matrix of order k are represented by $\mathbf{e}_k$ and $\mathbf{I}_k$, respectively. The Frobenius norm of a matrix M , [23], is denoted by $\|M\|_F$. If M is square, its determinant is denoted by $\det(M)$. The Euclidean norm for a vector $\mathbf{v}$ is denoted by $\|\mathbf{v}\|$. If $M = (m_{ij})$ and $N = (n_{ij})$ we denote by $|M| = (|m_{ij}|)$ and $M \leq N$ if $m_{ij} \leq n_{ij}$ for all (i, j) . For more basic notation we refer to [6].

The overview of the paper is the following: after the Introduction, Section 2 presents the *ABC* matrix and known bounds for its spectral radius (referred to as the *ABC* spectral radius) and its energy (referred to as the *ABC* energy). Additionally, new bounds for the spectral radius of connected graphs with respect to the *ABC* matrix are introduced. Moreover, upper bounds for the *ABC* energy for bipartite graphs are revisited. In Section 3, we recall the definition of *H*-join of a family of regular graphs

(as defined in [3]) and study its ABC spectrum. We present bounds for the ABC spectral radius of those graphs. Section 4 applies the results from the previous section to study the ABC spectral radius of certain caterpillar graphs and its ABC energy is discussed. Finally, Section 5 focuses on determining an upper bound for the ABC energy of the caterpillar $T(q, \dots, q)$.

2 The ABC matrix and bounds for its spectral radius and energy

The atom-bond connectivity matrix or ABC matrix of graph G of order n , $\Omega(G)$, [5, 6] is a type of combinatorial matrix constructed based on the adjacency matrix and the degree matrix of a graph as follows:

$$\Omega(G) = (\tau_{ij})_{1 \leq i, j \leq n}, \quad (3)$$

where

$$\tau_{ij} = \begin{cases} \sqrt{\frac{d_i + d_j - 2}{d_i d_j}} & \text{if } ij \in \mathcal{E}(G) \\ 0 & \text{otherwise.} \end{cases}$$

The matrix in (3) was designed as a weighted adjacency matrix of G , [5], and is commonly associated with the atom-bond connectivity index (see below). This matrix plays a crucial role in understanding the spectral properties of networks and graphs, as well as in modeling the dynamics of systems governed by such matrices.

The *atom-bond connectivity index* of a graph G , [10], is defined by

$$ABC(G) = \sum_{ij \in \mathcal{E}(G)} \sqrt{\frac{d_i + d_j - 2}{d_i d_j}}. \quad (4)$$

Ernesto Estrada et al. in [10] have proposed the index in (4) where it was simply called the ABC index. This invariant displays an excellent correlation with the heat of formation of alkanes [10, 11] and is of special importance in chemical graph theory as it gives information on the molecular structure of chemical compounds and is related to their biological

activity, chemical reactivity, and thermodynamic properties.

A connected graph is known as a *molecular* graph if its maximum degree is at most four. Furtula et al. [13] determined the minimum and maximum values of this index for molecular trees and showed that the star is the unique tree with the maximum *ABC* index when the number of vertices is given. Kinkar Ch. Das [7] presented lower and upper bounds on the *ABC* index of graphs and trees, and characterize graphs for which these bounds are the best possible. See also [17] and [8] for further reading.

We recall that the matrix $\Omega(G)$, is symmetric, thus its eigenvalues are real and can be ordered as follows: $\nu_1 \geq \nu_2 \geq \dots \geq \nu_n$. The set of the eigenvalues of the previous matrix is called *the ABC spectrum* of G and it is denoted by $\sigma_{ABC}(G)$. The spectral radius of the *ABC* matrix of G is called *the ABC spectral radius of G* and it is denoted by $\rho(\Omega(G))$. It is a global structural descriptor of a molecular graph and it reflects branching and degree distribution of the molecule.

2.1 Bounds for the spectral radius of the *ABC* matrix

In this subsection, we present several bounds for the *ABC* spectral radius, which have been identified in the literature. We also present some new bounds.

Theorem 1. [5] *If G is a connected graph without triangles of order $n \geq 3$, then*

$$\rho(\Omega(G)) \leq \sqrt{n-2},$$

with equality if and only if $G \cong K_{n_1, n_2}$ with $n_1 + n_2 = n$. Moreover, if G is a connected graph then

$$\min\{\sqrt{d_i + d_j - 2} : ij \in \mathcal{E}(G)\} \leq \rho(\Omega(G)) \leq \max\{\sqrt{d_i + d_j - 2} : ij \in \mathcal{E}(G)\},$$

with equality on both inequalities if and only if G is regular or bipartite semiregular.

The following corollary is a direct consequence of Theorem 1.

Corollary 1. [5] *Let G be a connected graph. Then*

$$\sqrt{2\delta(G) - 2} \leq \rho(\Omega(G)) \leq \sqrt{2\Delta(G) - 2},$$

with equality in both inequalities if and only if G is regular.

Concerning trees we also present some known results related with the ABC spectral radius.

Theorem 2. [6] *Let $\mathcal{T}$ be a tree of order $n \geq 3$. Then,*

$$\sqrt{2} \cos \frac{\pi}{n+1} \leq \rho(\Omega(\mathcal{T})) \leq \sqrt{n-2},$$

with equality on the left-hand side of the inequality if and only if $\mathcal{T} \cong P_n$, and equality on the right-hand side of the inequality if and only if $\mathcal{T} \cong S_n$.

Theorem 3. [6] *If G is a connected graph of order $n \geq 3$, then*

$$\sqrt{2} \cos \frac{\pi}{n+1} \leq \rho(\Omega(G)) \leq \sqrt{2n-4},$$

with equality on the left-hand side of the inequality if and only if $G \cong P_n$, and equality on the right-hand side of the inequality if and only if $G \cong K_n$.

2.2 Bounds for the energy of the ABC matrix

This subsection presents the definition of the ABC energy and some bounds established in the literature. Furthermore, we give new upper bounds for the ABC energy for bipartite graphs.

The energy of the ABC matrix associated to a graph G with n vertices (see [12]) is given by

$$E_{ABC}(G) = \sum_{i=1}^n |\nu_i|,$$

where ν_i is the i -th largest eigenvalue of $\Omega(G)$, $i = 1, \dots, n$.

Theorem 4. [4] *If $G = G_1 \cup G_2 \cup \dots \cup G_r$ then*

$$E_{ABC}(G) = \sum_{i=1}^r E_{ABC}(G_i).$$

Theorem 5. [4] Let G be a graph with $n \geq 3$ vertices and without isolated vertices. The following statement hold:

1. If $k \geq 2$ and G is k -regular, then

$$E_{ABC}(G) = \frac{\sqrt{2k-2}}{2} E(G),$$

where

$$E(G) = \sum_{i=1}^n |\lambda_i|,$$

and $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ are the elements of σ_G .

2. If G is (Δ, δ) -semiregular bipartite, then

$$E_{ABC}(G) = \frac{\sqrt{\Delta + \delta - 2}}{2} E(G),$$

in particular

$$E_{ABC}(K_{a,b}) = 2\sqrt{n-2}, \quad a+b=n.$$

The next result gives an upper bound for $E_{ABC}(G)$.

Theorem 6. [4] Let G be a graph without isolated vertices and order $n \geq 3$. Then

$$E_{ABC}(G) \leq n \sqrt{2 \left(1 - \frac{1}{\Delta(G)} \right)},$$

with equality if and only if $G \cong \frac{n}{2}K_2$. If $k \geq 2$ and G is a connected k -regular graph, then

$$E_{ABC}(G) \leq \sqrt{k} + \sqrt{(n-1)(n-k)} \sqrt{2 \left(1 - \frac{1}{k} \right)},$$

with equality if and only if $G \cong K_n$ or $G \cong \text{sr}g \left(n, k, \frac{k(k-1)}{n-1}, \frac{k(k-1)}{n-1} \right)$.

To establish an upper bound for the ABC energy in the context of bipartite graphs, we present some auxiliary results from [1, 15, 18].

Lemma 1. [15] Let G be a graph of order $n \geq 3$ without isolated vertices and ABC eigenvalues $\nu_1, \dots, \nu_n$. The following equalities hold:

1. $\sum_{i=1}^n \nu_i = 0$.
2. $\sum_{i=1}^n \nu_i^2 = 2n - 4R_{-1}(G)$,

where $R_{-1}(G)$ is defined in (1).

As recalled in [18, Chap 3], if a nonnegative irreducible square matrix M has a maximal eigenvalue r and exactly h eigenvalues of modulus r , then h is referred to as the index of imprimitivity of M . Furthermore, a symmetric irreducible nonnegative matrix M must have an imprimitivity index of 2. According to its Frobenius form ([18, Theorem 3.1]), there exists a permutation matrix P such that

$$M = P^T \begin{pmatrix} \mathbf{0} & \mathbf{M}_{12} \\ \mathbf{M}_{21} & \mathbf{0} \end{pmatrix} P, \quad (5)$$

where the zero blocks in the main diagonal are square.

The following result was proved in [1]:

Theorem 7. [1] Let M be an imprimitive symmetric nonnegative irreducible matrix whose Frobenius form is given in Eq (5). If M_{12} has order $m_1 \times m_2$, M_{21} has order $m_2 \times m_1$ and $\tilde{m} = \min\{m_1, m_2\}$, then

$$E(M) \leq 2\lambda_1(M) + 2\sqrt{(\tilde{m} - 1)(\|M\|_F^2/2 - \lambda_1^2(M))}. \quad (6)$$

Equality holds if and only if M has $2(\tilde{m} - 1)$ eigenvalues beyond $\pm\lambda_1(M)$ with the same modulus, namely $\sqrt{\frac{\|M\|_F^2/2 - \lambda_1^2(M)}{\tilde{m} - 1}}$ and $|m_2 - m_1|$ eigenvalues equal to 0.

Corollary 2. Let M be an imprimitive symmetric nonnegative irreducible matrix whose Frobenius form is given in Eq. (5). Let M_{12} and M_{21} matrices with orders $m_1 \times m_2$ and $m_2 \times m_1$ respectively, and $\tilde{m} = \min\{m_1, m_2\}$. If

$$\lambda_1(M) \geq \psi \geq \frac{\|M\|_F}{\sqrt{2\tilde{m}}}, \quad (7)$$

then

$$E(M) \leq 2\psi + 2\sqrt{(\tilde{m} - 1)(\|M\|_F^2/2 - \psi^2)}. \quad (8)$$

A value T in the condition (7) exists, and is neither equal to $\lambda_1(M)$ nor $\frac{\|M\|_F}{\sqrt{2\tilde{m}}}$, if and only if M has at least two eigenvalues with distinct modulus.

Proof. Consider

$$f(x) = x + \sqrt{(\tilde{m} - 1)(\|M\|_F^2/2 - x^2)},$$

whose derivative is

$$f'(x) = 1 - \frac{\sqrt{\tilde{m} - 1} x}{\sqrt{\|M\|_F^2/2 - x^2}},$$

which is non-increasing if and only if $x \geq \frac{\|M\|_F}{\sqrt{2\tilde{m}}}$. Next, we will show that $\lambda_1(M) \geq \frac{\|M\|_F}{\sqrt{2\tilde{m}}}$.

Clearly, the cardinality of the set

$$\sigma_0(M) = \{\lambda \in \sigma_M : \lambda \neq 0\}$$

is the rank of M , say m_0 . Since M and MM^T have the same rank we conclude that $m_0 \leq 2\tilde{m}$ and $\lambda_1^2(M) = \max\{\lambda^2 : \lambda \in \sigma_0(M)\}$.

As the maximum of a numerical set is greater than its average, and equality holds if and only if all the numbers are equal, we have

$$\lambda_1^2(M) \geq \|M\|_F^2/m_0 \geq \|M\|_F^2/2\tilde{m}, \quad (9)$$

and the equality holds if and only if all the eigenvalues have the same modulus, namely, $|\lambda| = \|M\|_F/\sqrt{2\tilde{m}}$. The result follows from Theorem 7 and by comparing $f(\lambda_1(M))$ and $f(\psi)$. ■

The following result is obtained by the direct application of Theorem 7 applied to $M = \Omega(G)$ and using Lemma 1.

Theorem 8. *Let G be a bipartite connected graph with $n \geq 3$ vertices and bipartition V_1 and V_2 where $|V_1| = n_1$ and $|V_2| = n_2$. Let $k = \min\{n_1, n_2\}$*

and $n = n_1 + n_2$. Then,

$$E_{ABC}(G) \leq 2\nu_1 + 2\sqrt{(k-1)(n-2R_{-1}(G)-\nu_1^2)}. \quad (10)$$

Equality holds if and only if G has $2(k-1)$ nonzero ABC eigenvalues distinct from $\pm\nu_1$ with the same modules and $|n_2 - n_1|$ eigenvalues equal to 0.

The following result is a direct consequence of Corollary 2.

Corollary 3. Let G be a graph bipartite connected graph with $n \geq 3$ vertices and bipartition V_1 and V_2 where $|V_1| = n_1$ and $|V_2| = n_2$. Let $k = \min\{n_1, n_2\}$ and $n = n_1 + n_2$. If $\nu_1 \geq \psi \geq \sqrt{\frac{n-2R_{-1}(G)}{k}}$. Then

$$E_{ABC}(G) \leq 2\psi + 2\sqrt{(k-1)(n-2R_{-1}(G)-\psi^2)}. \quad (11)$$

The following result uses Corollary 1.

Corollary 4. Let G be bipartite connected graph with $n > 3$ vertices and bipartition V_1 and V_2 where $|V_j| = k$, $j = 1, 2$. . If $n = 2k$ and $\delta \neq 1$, then

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

Proof. In the inequalities below, we take into account that $R_{-1}(G) \geq \frac{n}{2\Delta}$ (2). Note also that $(\delta-1)\Delta > \Delta-1$. Thus,

$$\begin{aligned} (\delta-1)\Delta &> \Delta-1 \\ \Leftrightarrow (\delta-1)\Delta+1 &> \Delta \\ \Leftrightarrow (\delta-1)k\Delta+k &> k\Delta \\ \Leftrightarrow (2\delta-2)k\Delta+n &> n\Delta \\ \Leftrightarrow (2\delta-2)k+\frac{n}{\Delta} &> n. \end{aligned}$$

Then,

$$\begin{aligned}
 (2\delta - 2)k + 2R_{-1}(G) &> n \\
 \Leftrightarrow 2\delta - 2 &> \frac{n - 2R_{-1}(G)}{k} \\
 \Leftrightarrow \sqrt{2\delta - 2} &> \sqrt{\frac{n - 2R_{-1}(G)}{k}},
 \end{aligned}$$

where this last inequality is the condition in the above result (Corollary 2.20). ■

3 The *ABC* spectrum of the *H*-join of graphs

The spectrum of the *H*-join of graphs, that is a generalized join operation on a family of graphs, regular in the case of the adjacency matrix and arbitrary in the case of the Laplacian matrix, was characterized in [3, Theorem 5]. In [3] this operation was designated by *H*-join of a family of graphs $G_1, \dots, G_k$, where *H* is an arbitrary graph of order *k*, but this definition is the same as the so called generalized composition, considered in [22] with the notation $H[G_1, \dots, G_k]$, where the adjacency spectra of $H[G_1, \dots, G_k]$, when $G_1, \dots, G_k$ are all regular, was also treated. Using almost equitable partitions [9], in [14] the Laplacian eigenvectors and eigenvalues of the *H*-join (generalized composition) of a family of graphs $G_1, \dots, G_k$ were determined, in particular, all the eigenvalues of each one of the graphs of the family with eigenspaces orthogonal to the all-one vector are also eigenvalues of the *H*-join. Following a different approach, the same result is proven in [3]. We recall here some of the definitions and results.

Let *H* be a graph with *k* vertices and without isolated vertices. Let $G_1, G_2, \dots, G_k$ be a finite family of p_j -regular graphs, with vertex sets $V(G_j)$, for $j = 1, \dots, k$ which are pairwise disjoint. Moreover, suppose that the graphs G_j have n_j vertices for $j = 1, \dots, k$. Let $G \cong H[G_1, \dots, G_k]$. Let A_j be the adjacency matrix of G_j , $j = 1, \dots, k$. Let $A_H = (\delta_{ij})_{1 \leq i, j \leq n}$

be the adjacency matrix of H . Consider the matrix $\widehat{C}$ below, called the *quotient matrix* of the H -join:

$$\widehat{C} = \begin{pmatrix} p_1 & \delta_{12}\sqrt{n_1n_2} & \cdots & \delta_{1k}\sqrt{n_1n_k} \\ \delta_{12}\sqrt{n_2n_1} & p_2 & \ddots & \delta_{2k}\sqrt{n_2n_k} \\ \vdots & & \ddots & \vdots \\ \vdots & & \ddots & \vdots \\ \delta_{k1}\sqrt{n_kn_1} & \cdots & \delta_{k(k-1)}\sqrt{n_kn_{k-1}} & p_k \end{pmatrix}. \quad (12)$$

Applying [3, Theorem 3], the following result, that relates the spectrum of the adjacency matrix of the H -join and the matrix in (12), is obtained.

Theorem 9. [3] For $j = 1, 2, \dots, k$ let G_j be a p_j -regular graph with n_j vertices and spectrum σ_j . If $G \cong H[G_1, \dots, G_k]$ and $\widehat{C}$ is the matrix in (12), then

$$\sigma_G = \sigma_{\widehat{C}} \cup \bigcup_{j=1}^k \sigma_j \setminus \{p_j\}.$$

Applying again [3, Theorem 3] we obtain an analogous result for the ABC -matrix of the H -join of k disjoint regular graphs.

To define the ABC matrix associated with the H -join, it is crucial to establish key invariants related to the H -join of graphs, which can be found in [3].

Definition 1. For $j = 1, 2, \dots, k$ let G_j be a p_j regular graph with n_j vertices and spectrum σ_j . Let $G \cong H[G_1, \dots, G_k]$ and

$$N_j = \sum_{ij \in \mathcal{E}(H)} n_i. \quad (13)$$

Note that the degree of an arbitrary vertex $v \in \mathcal{V}(G_j)$, as vertex of G , is

$p_j + N_j$. Let

$$\beta_j = \frac{\sqrt{2}\sqrt{p_j + N_j - 1}}{p_j + N_j}. \quad (14)$$

Consider the matrix

$$\tilde{\Omega}(G_j) = \beta_j A(G_j), j = 1, \dots, k. \quad (15)$$

Let ρ be the following $\frac{k(k-1)}{2}$ -tuple of scalars

$$\rho = (\rho_{12}, \dots, \rho_{1k}, \rho_{23}, \dots, \rho_{2k}, \dots, \rho_{k-1,k}) \quad (16)$$

such that

$$\rho_{ij} = \delta_{ij} \sqrt{\frac{(p_i + p_j + N_i + N_j - 2)n_i n_j}{(p_i + N_i)(p_j + N_j)}}. \quad (17)$$

Thus, the ABC matrix of the H -join $H[G_1, \dots, G_k]$ is:

$$\Omega(G) = \begin{pmatrix} \tilde{\Omega}(G_1) & \frac{\rho_{12}\mathbf{e}_{n_1}\mathbf{e}_{n_2}^T}{\sqrt{n_1 n_2}} & \dots & \dots & \frac{\rho_{1k}\mathbf{e}_{n_1}\mathbf{e}_{n_k}^T}{\sqrt{n_1 n_k}} \\ \frac{\rho_{12}\mathbf{e}_{n_1}\mathbf{e}_{n_2}^T}{\sqrt{n_1 n_2}} & \tilde{\Omega}(G_2) & \frac{\rho_{23}\mathbf{e}_{n_2}\mathbf{e}_{n_3}^T}{\sqrt{n_2 n_3}} & \dots & \vdots \\ \vdots & \frac{\rho_{23}\mathbf{e}_{n_2}\mathbf{e}_{n_3}^T}{\sqrt{n_2 n_3}} & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ \frac{\rho_{1k}\mathbf{e}_{n_1}\mathbf{e}_{n_k}^T}{\sqrt{n_1 n_k}} & \dots & \dots & \frac{\rho_{k-1,k}\mathbf{e}_{n_{k-1}}\mathbf{e}_{n_k}^T}{\sqrt{n_{k-1} n_k}} & \tilde{\Omega}(G_k) \end{pmatrix} \quad (18)$$

Moreover, the matrix

$$\hat{\Omega}(G) = \begin{pmatrix} \beta_1 p_1 & \rho_{12} & \dots & \dots & \rho_{1k} \\ \rho_{12} & \beta_2 p_2 & \rho_{23} & \dots & \vdots \\ \vdots & \rho_{23} & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ \rho_{1k} & \dots & \dots & \rho_{k-1,k} & \beta_k p_k \end{pmatrix}. \quad (19)$$

is called the ABC quotient matrix of the H -join.

The following result characterize the ABC spectrum of an H -join of regular graphs.

Theorem 10. Let $A(H) = (\delta_{ij})_{1 \leq i, j \leq k}$. For $1 \leq j \leq k$ let G_j be a p_j -regular graph with n_j vertices. Consider the vector in (16) defined as (17). Let σ_j be the spectrum of graph G_j , $j = 1, \dots, k$. Consider N_j be the integer defined as (13). Then,

$$\sigma_{ABC}(G) = \sigma_{\hat{\Omega}(G)} \cup \bigcup_{j=1}^k \left\{ \frac{\sqrt{2}\sqrt{p_j + N_j - 1}}{p_j + N_j} \lambda : \lambda \in \sigma_j \setminus \{p_j\} \right\}$$

where $\hat{\Omega}(G)$ is the matrix in (19). In particular, if $G_j \cong \overline{K}_{n_j}$, $j = 1, \dots, k$, we obtain

$$\sigma_{ABC}(G) = \{0^{[n-k]}\} \cup \sigma_{\hat{\Omega}(G)}$$

where

$$\hat{\Omega}(G) = \begin{pmatrix} 0 & \rho_{12} & \cdots & & \rho_{1k} \\ \rho_{12} & 0 & \rho_{23} & \cdots & \vdots \\ \vdots & \rho_{23} & \ddots & \ddots & \\ & & \ddots & \ddots & \rho_{k-1,k} \\ \rho_{1k} & \cdots & & \rho_{k-1,k} & 0 \end{pmatrix} \quad (20)$$

and

$$\rho_{ij} = \delta_{ij} \sqrt{\frac{n_i n_j}{N_i N_j}} \sqrt{N_i + N_j - 2}, \quad (21)$$

for all $1 \leq i \leq k-1$ and $2 \leq j \leq k$, n_i is the number of vertices of G_i and N_i is the invariant defined in (13).

Theorem 11. Let G_j be a connected p_j -regular graph, with $j = 1, 2, \dots, k$. The ABC spectral radius of the H-join $G \cong H[G_1, \dots, G_k]$, with H connected, and the spectral radius of the matrix $\hat{\Omega}(G)$ in (19) coincide.

Proof. Firstly, it is important to observe that both matrices $\hat{\Omega}(G)$ in (19) and $\Omega(G)$ in (18) are nonnegative irreducible matrices. Therefore, the eigenvectors corresponding to their largest eigenvalues have (up to a negative scalar multiple) all coordinates positive, [18, Corollary 4.2]. On the other hand, by [18, Theorem 4.4] we can conclude that the maximal eigenvalue of a nonnegative irreducible matrix M is the unique eigenvalue of M that has an associated positive eigenvector (up to a negative scalar

multiple). From the proof of the result [3, Theorem 3], it is clear that the eigenvectors associated to the eigenvalues of $\Omega(G)$, which come from the eigenvalues of $\widehat{\Omega}(G)$, are constructed by the product of the coordinates of the respective eigenvector of $\widehat{\Omega}(G)$ and the vector $\mathbf{v} = (\mathbf{v}_1^T, \mathbf{v}_2^T, \dots, \mathbf{v}_k^T)^T$ with $\widetilde{\Omega}(G_j) \mathbf{v}_j = \beta_j p_j \mathbf{v}_j, \forall j$, where $\widetilde{\Omega}(G)$ is the matrix in (15) and β_j are the elements in (14). Since, for all j , $\mathbf{v}_j$ is a maximal eigenvector and $\widetilde{\Omega}(G_j)$ is a nonnegative irreducible matrix, $\mathbf{v}_j$ is positive (up to a negative scalar multiple). Taking into account the products among the positive coordinates of the maximal eigenvector of $\widehat{\Omega}(G)$ and the vector components of the vector $\mathbf{v}$ the result follows. ■

4 Application to the ABC spectrum of caterpillars

In chemical graph theory, caterpillar trees are widely used. A caterpillar tree represents a benzenoid hydrocarbon molecule allowing a better prediction and analysis of its properties, stability and reactivity. We label the vertices of the caterpillar $T(q_1, \dots, q_r)$ with $q_i \geq 1$, in the following form:

1. The labels $1, \dots, r$ are used in the path P_r from left to right.
2. Again, from left to right the labels $r + i$ con $1 \leq i \leq n - r$ are used in the $q_1 + q_2 + \dots + q_r$ pendant vertices of $T(q_1, \dots, q_r)$.
3. Let $H_0 \cong T(1, 1, \dots, 1)$. Then H_0 is a graph of order $2r$. Using the labeling for the vertices described in 1. and 2., the adjacency matrix of H_0 is the following block matrix:

$$A(H_0) = \begin{pmatrix} A(P_r) & I_r \\ I_r & \mathbf{O} \end{pmatrix}. \quad (22)$$

After labeling the vertices of the caterpillar we note that,

$$G \cong T(q_1, \dots, q_r) = H_0 [\overline{K}_1, \dots, \overline{K}_1, \overline{K}_{q_1}, \dots, \overline{K}_{q_r}].$$

Here $\overline{K}_1$ appears r times, the vertices 1 and r of the path P_r have $1 + q_1, 1 + q_r$ neighbors, respectively. Meanwhile, the vertices from 2 to $r - 1$ of P_r have $q_2 + 2, q_3 + 2, \dots, q_{r-1} + 2$ neighbors, respectively.

4. Moreover, $n_1 = n_2 = \dots = n_r = 1$, $n_{1+r} = q_1$, $n_{2+r} = q_2, n_{3+r} = q_3, \dots, n_{2r} = q_r$, and $p_j = 0$ for all $1 \leq j \leq 2r$.
5. For the graph $H_0 [\overline{K}_1, \dots, \overline{K}_1, \overline{K}_{q_1}, \dots, \overline{K}_{q_r}]$ the invariants given by Definition 1 are

- (a) $N_1 = q_1 + 1$, and $N_r = 1 + q_r$,
- (b) $N_j = 2 + q_j$ ($2 \leq j \leq r - 1$) and,
- (c) $N_{r+1} = 1 = N_{2+r} = \dots = N_{2r}$.

The entries defined in (21) of the corresponding quotient matrix are: $\rho_{ij} = 0$ if $j \notin \{i + 1, r + i\}$, and $\forall 1 \leq i \leq r - 1$. Additionally,

$$\rho_{i(i+r)} = \begin{cases} \frac{q_i}{\sqrt{q_i + 1}} & \text{if } i = 1 \text{ or } i = r \\ \sqrt{q_i \frac{q_i + 1}{q_i + 2}} & \text{if } 2 \leq i \leq r - 2, \end{cases}$$

and

$$\rho_{i(i+1)} = \begin{cases} \sqrt{\frac{q_i + q_{i+1} + 1}{(q_i + 1)(q_{i+1} + 2)}} & \text{if } i = 1 \\ \sqrt{\frac{q_i + q_{i+1} + 1}{(q_i + 2)(q_{i+1} + 1)}} & \text{if } i = r - 1 \\ \sqrt{\frac{q_i + q_{i+1} + 2}{(q_i + 2)(q_{i+1} + 2)}} & \text{if } 2 \leq i \leq r - 2. \end{cases}$$

In order to present the ABC quotient matrix of the H_0 -join, $\widehat{\Omega}_0(G)$, we note that its entries are zero where the entries of $A(H_0)$, in (22), are zero.

Thus,

$$\widehat{\Omega}_0(G) = \begin{pmatrix} \Lambda(P_r)(G) & \Upsilon_r(G) \\ \Upsilon_r(G) & \mathbf{O}_r \end{pmatrix},$$

where the submatrices $\Upsilon_r = \Upsilon_r(G)$ are diagonal matrices such that

$$\begin{aligned}\Upsilon_r &= \text{diag} \left(\rho_{1(1+r)} \quad \rho_{2(2+r)} \quad \cdots \quad \rho_{(r-1)(2r-1)} \quad \rho_{r(2r)} \right) \\ &= \text{diag} \left(\frac{q_1}{\sqrt{q_1+1}} \quad \sqrt{q_2 \frac{q_2+1}{q_2+2}} \quad \cdots \quad \sqrt{q_{r-1} \frac{q_{r-1}+1}{q_{r-1}+2}} \quad \frac{q_r}{\sqrt{q_r+1}} \right) \quad (23)\end{aligned}$$

and $\Lambda = \Lambda(P_r)(G)$ is:

$$\Lambda = \begin{pmatrix} 0 & \sqrt{\frac{q_1+q_2+1}{(1+q_1)(2+q_2)}} & 0 & \cdots & & 0 \\ \sqrt{\frac{q_1+q_2+1}{(1+q_1)(2+q_2)}} & 0 & \sqrt{\frac{q_2+q_3+2}{(q_2+2)(q_3+2)}} & & 0 & \vdots \\ 0 & \sqrt{\frac{q_2+q_3+2}{(q_2+2)(q_3+2)}} & 0 & \sqrt{\frac{q_3+q_4+2}{(q_3+2)(q_4+2)}} & & \\ & \ddots & \ddots & \ddots & \ddots & \\ \vdots & & \ddots & & \ddots & \\ & & & \sqrt{\frac{q_{r-2}+q_{r-1}+2}{(q_{r-2}+2)(q_{r-1}+2)}} & 0 & \\ & & \sqrt{\frac{q_{r-2}+q_{r-1}+2}{(q_{r-2}+2)(q_{r-1}+2)}} 0 & \sqrt{\frac{q_{r-1}+q_r+1}{(q_{r-1}+2)(q_r+1)}} & & \\ 0 & \cdots & & \sqrt{\frac{q_{r-1}+q_r+1}{(q_{r-1}+2)(q_r+1)}} & 0 & \end{pmatrix}. \quad (24)$$

Sometimes, to simplify notation we just use $\Lambda(P_r)(G) = \Lambda(P_r)$.

Proposition 12. *Let $r \geq 3$. Consider the caterpillar $G \cong T(q_1, \dots, q_r)$. Let*

$$\begin{aligned}\mathbf{m} &= \min \left\{ \sqrt{q_1}, \sqrt{q_r}, \sqrt{q_j+1} : 2 \leq j \leq r-1 \right\}, \text{ and} \\ \mathbf{M} &= \max \left\{ \sqrt{1+q_1+q_2}, \sqrt{1+q_{r-1}+q_r}, \sqrt{q_j+q_{j+1}+2} : 2 \leq j \leq r-2 \right\}.\end{aligned}$$

Then,

$$\mathbf{m} \leq \rho(\Omega(G)) \leq \mathbf{M}.$$

Proof. In [2], the quotient matrix Θ_{2r} of the Randić matrix of the caterpillar $T(q_1, \dots, q_r)$, viewed as an H -join, is the matrix of order $2r \times 2r$ given by:

$$\Theta_{2r} = \begin{pmatrix} A & B \\ C & D \end{pmatrix},$$

where $A = (a_{ij})$ is the symmetric matrix where the entries above the principal diagonal are:

$$\begin{aligned} a_{12} &= \frac{1}{\sqrt{(1+q_1)(2+q_2)}}, \\ a_{i,i+1} &= \frac{1}{\sqrt{(2+q_i)(2+q_{i+1})}}, i \in \{2, \dots, r-2\} \\ a_{r-1,r} &= \frac{1}{\sqrt{(1+q_r)(2+q_{r-1})}}, \end{aligned}$$

and all the other entries are equal to zero. Moreover,

$B = C = \text{diag} \left(\sqrt{\frac{q_1}{q_1+1}}, \sqrt{\frac{q_2}{q_2+2}}, \dots, \sqrt{\frac{q_{r-1}}{q_{r-1}+2}}, \sqrt{\frac{q_r}{q_r+1}} \right)$ and D is the null matrix of appropriate order.

The ABC quotient matrix of the caterpillar $G \cong T(q_1, \dots, q_r)$, is a matrix in the form:

$$\widehat{\Omega}_0(G) = \begin{pmatrix} A^* & B^* \\ C^* & D^* \end{pmatrix}$$

Where $A^* = (a_{ij}^*)$ is the symmetric matrix where the entries above the principal diagonal are:

$$\begin{aligned} a_{12}^* &= \sqrt{\frac{q_1 + q_2 + 1}{(1+q_1)(2+q_2)}}, \\ a_{i,i+1}^* &= \sqrt{\frac{q_i + q_{i+1} + 2}{(2+q_{i+1})(q_3+2)}}, i \in \{2, \dots, r-2\} \\ a_{r-1,r}^* &= \sqrt{\frac{q_{r-1} + q_r + 1}{(1+q_r)(2+q_{r-1})}} \end{aligned}$$

and all the other entries are equal to zero. Moreover $B^* = C^*$ are equal to

$$\text{diag} \left(\sqrt{q_1} \sqrt{\frac{q_1}{q_1+1}}, \sqrt{1+q_2} \sqrt{\frac{q_2}{q_2+2}}, \dots, \sqrt{1+q_{r-1}} \sqrt{\frac{q_{r-1}}{q_{r-1}+2}}, \sqrt{q_r} \sqrt{\frac{q_r}{q_r+1}} \right),$$

and D^* is the null matrix of appropriate order.

It is clear that

$$\mathbf{m}\Theta_{2r} \leq \widehat{\Omega}_0(T(q_1, \dots, q_r)) \leq \mathbf{M}\Theta_{2r}.$$

Thus, we have

$$\mathbf{m} \leq \rho\left(\widehat{\Omega}_0(T(q_1, \dots, q_r))\right) \leq \mathbf{M},$$

as the largest eigenvalue of Θ_{2r} is equal to 1. ■

The following result show that the upper bound obtained in Proposition 12 is not worse than the upper bound of Corollary 1.

Proposition 13. *The upper bound obtained in Proposition 12 is not worse than the upper bound given in Corollary 1.*

Proof. If $\Delta \in \{q_1 + 1, q_r + 1\}$, without loss of generality we suppose that $q_1 \geq q_r$ and $\Delta = 1 + q_1$. Thus, $2\Delta - 2 = 2q_1$. Moreover

$$q_1 \geq q_j + 1, j = 2, \dots, r - 1.$$

Therefore,

$$2q_1 \geq q_j + q_{j+1} + 2, j = 1, \dots, r - 1.$$

In particular,

$$2q_1 \geq q_1 + q_2 + 1$$

and

$$2q_1 \geq q_r + q_{r-1} + 1.$$

Then,

$$\begin{aligned} \mathbf{M} &= \max \left\{ \sqrt{1 + q_1 + q_2}, \sqrt{1 + q_{r-1} + q_r}, \sqrt{q_j + q_{j+1} + 2}, 2 \leq j \leq r - 2 \right\} \\ &\leq \sqrt{2\Delta - 2}. \end{aligned}$$

If $\Delta = q_{j_0} + 2$ then $q_{j_0} \geq q_j$, $\forall 2 \leq j \leq r - 1$ and $q_{j_0} \geq q_{j+1}$, $\forall 1 \leq j \leq r - 2$. Then,

$$2\Delta - 2 = 2q_{j_0} + 2 \geq q_j + q_{j+1} + 2 \quad \forall 2 \leq j \leq r - 2.$$

Moreover, $q_{j_0} \geq q_1 - 1$ and $q_{j_0} \geq q_r - 1$. Thus, $2q_{j_0} + 2 \geq q_1 + q_2 + 1$ and $2q_{j_0} + 2 \geq q_r + q_{r-1} + 1$, which proves the statement. $\blacksquare$

Remark. The upper bound in Proposition 12 is the upper bound in Theorem 1 except that the former does not take into account the pendant vertices.

In what follows we search for an upper bound for the ABC spectral radius of the particular caterpillar $T(q, q, \dots, q)$ that improves the upper bound in Corollary 1. Let

$$\lambda_1(\Lambda(P_r)) \geq \lambda_2(\Lambda(P_r)) \geq \dots \geq \lambda_r(\Lambda(P_r)),$$

the eigenvalues $\Lambda(P_r)$.

When $q_1 = q_2 = \dots = q_r = q$, the matrix $\Lambda(P_r)$ is:

$$\Lambda(P_r) = \begin{pmatrix} 0 & \sqrt{\frac{2q+1}{(1+q)(2+q)}} & 0 & \dots & & 0 \\ \sqrt{\frac{2q+1}{(1+q)(2+q)}} & 0 & \frac{\sqrt{2+2q}}{2+q} & & 0 & \vdots \\ 0 & \frac{\sqrt{2+2q}}{2+q} & \ddots & \frac{\sqrt{2+2q}}{2+q} & & \vdots \\ & & \ddots & \ddots & \ddots & \vdots \\ \vdots & & & \ddots & \ddots & \vdots \\ & & & & \frac{\sqrt{2+2q}}{2+q} & 0 \\ & & & \frac{\sqrt{2+2q}}{2+q} & 0 & \sqrt{\frac{2q+1}{(1+q)(2+q)}} \\ 0 & \dots & & \sqrt{\frac{2q+1}{(1+q)(2+q)}} & 0 \end{pmatrix} \quad (25)$$

and

$$\Upsilon_r = \text{diag}\left(\frac{q}{\sqrt{q+1}} \quad \sqrt{q\frac{q+1}{q+2}} \quad \dots \quad \sqrt{q\frac{q+1}{q+2}} \quad \frac{q}{\sqrt{q+1}}\right). \quad (26)$$

Thus,

$$\hat{\Omega}_0 = \begin{pmatrix} \Lambda(P_r) & \Upsilon_r \\ \Upsilon_r & \mathbf{O}_r \end{pmatrix}, \quad (27)$$

is the ABC quotient matrix in this case.

The following lower bound for $\tilde{\nu}_1(q)$ is rapidly obtained.

Lemma 2. *Let $\tilde{\nu}_1(q)$ be the ABC spectral radius of the caterpillar $G \cong T(q, \dots, q)$ where q is repeated r times. If Φ is equal to*

$$4 \left(\frac{q}{q+1} \sqrt{\frac{2q+1}{(q+2)}} + \frac{\vartheta}{(q+2)^{\frac{3}{2}}} \right), \quad (28)$$

with

$$\vartheta = \sqrt{4q+2} + \sqrt{2q} + \sqrt{2q^{\frac{3}{2}}} + \sqrt{2q^3 + 5q^2 + 2q} + \sqrt{2q}(r-4)(q+1),$$

and

$$\xi(q) = \sqrt{\frac{2rq^3 + 6rq^2 + 12rq + 8r - 24q - 20}{2r(q+2)^2} + \frac{\Phi}{2r}}, \quad (29)$$

then

$$\xi(q) \leq \tilde{\nu}_1(q).$$

Proof. The proof follows from a well known inequality $\frac{\mathbf{e}^T M^2 \mathbf{e}}{2r} \leq \tilde{\nu}_1^2(q)$, where $\mathbf{e}$ is the $2r$ -dimensional all ones vector and $M = \widehat{\Omega}_0(G)$. From the equality $\mathbf{e}^T M^2 \mathbf{e} = \|M\mathbf{e}\|^2$ and considering that

$$\sqrt{\frac{\mathbf{e}^T M^2 \mathbf{e}}{2r}} = \xi(q), \quad (30)$$

we first compute $M\mathbf{e}$. Thus,

$$M\mathbf{e} = \begin{pmatrix} \sqrt{\frac{2q+1}{(q+1)(q+2)}} + \frac{q}{\sqrt{q+1}} \\ \sqrt{\frac{2q+1}{(q+1)(q+2)}} + \sqrt{q\frac{q+1}{q+2}} + \sqrt{2}\frac{\sqrt{q+1}}{q+2} \\ \sqrt{q\frac{q+1}{q+2}} + 2\sqrt{2}\frac{\sqrt{q+1}}{q+2} \\ \vdots \\ \sqrt{q\frac{q+1}{q+2}} + 2\sqrt{2}\frac{\sqrt{q+1}}{q+2} \\ \sqrt{\frac{2q+1}{(q+1)(q+2)}} + \sqrt{q\frac{q+1}{q+2}} + \sqrt{2}\frac{\sqrt{q+1}}{q+2} \\ \sqrt{\frac{2q+1}{(q+1)(q+2)}} + \frac{q}{\sqrt{q+1}} \\ \frac{q}{\sqrt{q+1}} \\ \sqrt{q\frac{q+1}{q+2}} \\ \vdots \\ \sqrt{q\frac{q+1}{q+2}} \\ \frac{q}{\sqrt{q+1}} \end{pmatrix}.$$

Therefore, if Φ is as in (28),

$$\|M\mathbf{e}\|^2 = \frac{2rq^3 + 6rq^2 + 12rq + 8r - 24q - 20}{(q+2)^2} + \Phi.$$

Thus

$$\frac{\|M\mathbf{e}\|}{\sqrt{2r}} = \xi(q) = \sqrt{\frac{2rq^3 + 6rq^2 + 12rq + 8r - 24q - 20}{2r(q+2)^2} + \frac{\Phi}{2r}},$$

and the statement follows. ■

4.1 Upper bound for the ABC energy of certain caterpillars

In this section, we provide an upper bound for the ABC energy of the caterpillar graph $T(q, \dots, q)$, along with a comparative table that contrasts this bound with the one presented in Theorem 6.

The following result uses Corollary 2 and Lemma 2 to establish an upper bound for the energy of the caterpillar graph $G \cong T(q, q, \dots, q)$.

To achieve this, we must verify the condition in (7) for $T = \xi(q)$ and $M = \widehat{\Omega}_0(G)$.

Proposition 14. *Consider the graph $G \cong T(q, q, \dots, q)$, with q repeated $r \geq 3$ times. Let Φ and $\xi(q)$ defined in (28) and (29), respectively. Then,*

$$E_{ABC}(G) \leq 2\xi(q) + 2\sqrt{(r-1)\Gamma},$$

$$\text{where } \Gamma = \left(\frac{r(q^3+3q^2+4q+2)-q^3-3q^2-10q^2-6}{(q+2)^2} + \frac{24q+20}{2r(q+2)^2} - \frac{\Phi}{2r} \right).$$

Proof. Consider G as in the statement and $\xi(q)$ as defined in Lemma 2.

Claim: For all q ,

$$\xi(q) \geq \frac{\|\widehat{\Omega}_0(G)\|_F}{\sqrt{2r}}.$$

Proof of Claim: Let $M = \widehat{\Omega}_0(G)$ then is clear that the following inequality proceeds

$$\text{trace}(M^*M) \leq \mathbf{e}^T M^* M \mathbf{e}.$$

As $\|M\|_F^2 = \text{trace}(M^*M)$ and $M^* = M$ then the *Claim* follows. Taking into account the previous inequality, dividing by $2r$ and taking the square root, one obtain:

$$\frac{\|M\|_F}{\sqrt{2r}} \leq \sqrt{\frac{\mathbf{e}^T M^2 \mathbf{e}}{2r}} = \xi(q). \quad (31)$$

By Lemma 2, we see that $\xi(q)$ satisfies the conditions of ψ in the inequality in (7). Finally, by Corollary 2, the inequality is obtained. Now we compute the Frobenius norm of the matrix:

$$M = \widehat{\Omega}_0(G) = \begin{pmatrix} \Lambda(P_r) & \Upsilon_r \\ \Upsilon_r & \mathbf{O}_r \end{pmatrix}. \quad (32)$$

It is clear that,

$$\left\| \widehat{\Omega}_0(G) \right\|_F^2 = \|\Lambda(P_r)\|_F^2 + 2\|\Upsilon_r\|_F^2, \quad (33)$$

where $\Lambda(P_r)$ and Υ_r are defined in (25) and in (23), respectively. By the symmetry of $\Lambda(P_r)$ and Υ_r we see that

$$\|\Lambda(P_r)\|_F^2 = 2 \left(\frac{1+q_1+q_2}{(1+q_1)(2+q_2)} + \frac{1+q_{r-1}+q_r}{(1+q_r)(2+q_{r-1})} + \sum_{\ell=2}^{r-2} \frac{2+q_\ell+q_{\ell+1}}{(2+q_\ell)(2+q_{\ell+1})} \right)$$

and

$$\|\Upsilon_r\|_F^2 = \frac{q_1^2}{1+q_1} + \frac{q_r^2}{1+q_r} + \sum_{\ell=2}^{r-1} \frac{q_\ell(1+q_\ell)}{2+q_\ell}.$$

If $q_1 = q_2 = \dots = q_r = q$, then

$$\begin{aligned} \|\Lambda(P_r)\|_F^2 &= 2 \left(\frac{2+4q}{(1+q)(2+q)} + \sum_{\ell=2}^{r-2} \frac{2+2q}{(2+q)^2} \right) \\ &= 4 \left(\frac{1+2q}{(1+q)(2+q)} + \frac{(1+q)(r-3)}{(2+q)^2} \right), \end{aligned} \quad (34)$$

and

$$\|\Upsilon_r\|_F^2 = \frac{2q^2}{1+q} + \frac{q(1+q)}{2+q}(r-2). \quad (35)$$

We now compute the difference

$$\frac{\|\widehat{\Omega}_0(G)\|_F^2}{2} - \xi(q)^2 = \frac{\|\widehat{\Omega}_0(G)\|_F^2}{2} - \frac{\|M\mathbf{e}\|^2}{2r},$$

where

$$\begin{aligned} \frac{\|\widehat{\Omega}_0(G)\|_F^2}{2} &= 2 \left(\frac{1+2q}{(1+q)(2+q)} + \frac{(1+q)(r-3)}{(q+2)^2} \right) \\ &\quad + \frac{2q^2}{q+1} + \frac{q(q+1)}{q+2}(r-2) \end{aligned}$$

and

$$\frac{\|M\mathbf{e}\|^2}{2r} = \frac{2rq^3 + 6rq^2 + 12rq + 8r - 24q - 20}{2r(q+2)^2} + \frac{\Phi}{2r}.$$

Thus,

$$\begin{aligned} \frac{\|\widehat{\Omega}_0(G)\|_F^2}{2} - \frac{\|Me\|^2}{2r} &= \frac{r(q^3 + 3q^2 + 4q + 2) - q^3 - 3q^2 - 10q^2 - 6}{(q+2)^2} \\ &+ \frac{24q + 20}{2r(q+2)^2} - \frac{\Phi}{2r}. \end{aligned}$$

Using Corollary 2 the result follows. ■

Remark. For the caterpillar graph $T(q, q, \dots, q)$, the upper bound in Proposition 14 improves the upper bound in Theorem 6 which is equal to $r(1+q)\sqrt{\frac{2(q+1)}{q+2}}$. The explanation of this fact follows from [1, Lemma 3], which provides a tighter bound for the energy ABC by applying the Cauchy-Schwarz inequality to a portion of the summand involving the absolute values of the eigenvalues. In contrast, the bound in Theorem 6 is derived by applying the Cauchy-Schwarz inequality directly to the entire sum that defines the ABC energy, along with the left inequality in (2).

Example 1. The following comparative table, generated using MATLAB, presents the ABC energy ($E_{ABC}(G)$) and the upper bounds from Theorem 6 and Proposition 14 for a graph $G \cong T(q, q, \dots, q)$, across different values of r and q .

r	q	$E_{ABC}(G)$	Th 6	Prop 14
3	3	8.5629	15.1789	8.8882
3	4	9.9209	19.3649	10.2596
5	6	18.4484	46.3006	19.4371
7	8	27.6012	84.5234	29.3509
9	12	39.7378	159.4441	42.5442
3	12	17.0235	53.1480	17.7063
12	3	31.9057	60.7157	35.2771

Acknowledgment: We sincerely thank the referee for the constructive feedback and for highlighting additional relevant references, which have helped improve the quality and context of this work.

Enide Andrade is supported by CIDMA (<https://ror.org/05pm2mw36>) under the Portuguese Foundation for Science and Technology

(FCT, <https://ror.org/00snfq58>), Grants

UID/04106/2025 (<https://doi.org/10.54499/UID/04106/2025>)

UID/PRR/04106/2025

(<https://doi.org/10.54499/UID/PRR/04106/2025>)

References

- [1] M. Aguieiras, M. Robbiano, A. Bonifácio, An improved upper bound of the energy of some graphs and matrices, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 307–320.
- [2] E. Andrade, H. Gomes, M. Robbiano, Spectra and Randić spectra of caterpillar graphs and applications to the energy, *MATCH Commun. Math. Comput. Chem.* **77** (2017) 61–75.
- [3] D. M. Cardoso, M. A. de Freitas, E. A. Martins, M. Robbiano, Spectra of graphs obtained by a generalization of the join graph operation, *Discr. Math.* **313** (2013) 733–741.
- [4] X. Chen, On *ABC* eigenvalues and *ABC* energy, *Lin. Algebra Appl.* **544** (2018) 141–157.
- [5] X. Chen, A note on the *ABC* spectral radius of graphs, *Lin. Multilin. Algebra* **70** (2020) 775–786.
- [6] X. Chen, On extremality of *ABC* spectral radius of a tree, *Lin. Algebra Appl.* **564** (2019) 159–169.
- [7] K. C. Das, Atom–bond connectivity index of graphs, *Discr. Appl. Math.* **158** (2010) 1181–1188.
- [8] K. C. Das, I. Gutman, B. Furtula, On atom-bond connectivity index, *Chem. Phys. Lett.* **511** (2011) 452–454.
- [9] D. M. Cardoso, C. Delorme, P. Rama, Laplacian eigenvectors and eigenvalues and almost equitable partitions, *Eur. J. Comb.* **28** (2007) 665–673.
- [10] E. Estrada, L. Torres, L. Rodríguez, I. Gutman, An atom-bond connectivity index: Modelling the enthalpy of formation of alkanes, *Indian J. Chem.* **37A** (1998) 849–855.

-
- [11] E. Estrada, Atom–bond connectivity and the energetic of branched alkanes, *Chem. Phys. Lett.* **463** (2008) 422–425.
 - [12] E. Estrada, The *ABC* matrix, *J. Math. Chem.* **55** (2017) 1021–1033.
 - [13] B. Furtula, A. Graovac, D. Vukičević, Atom–bond connectivity index of trees, *Discr. Appl. Math.* **157** (2009) 2828–2835.
 - [14] A. Gerbaud, Spectra of generalized compositions of graphs and hierarchical networks, *Discr. Math.* **310** (2010) 2824–2830.
 - [15] M. Ghorbani, X. Li, M. Hakimi-Nezhaad, J. Wang, Bounds on the *ABC* spectral radius and *ABC* energy of graphs, *Lin. Algebra Appl.* **598** (2020) 145–164.
 - [16] I. Gutman, Topological properties of benzenoid systems. An identity for the sextet polynomial, *Theor. Chim. Acta* **45** (1977) 309–315.
 - [17] H. Hua, K. Das, H. Wang, On atom-bond connectivity index of graphs, *J. Math. Anal. Appl.* **479** (2019) 1099–1114.
 - [18] H. Minc, *Nonnegative Matrices*, Wiley, New York, 1988.
 - [19] D. B. West, *Introduction to Graph Theory*, Prentice-Hall, Englewood Cliffs, 2000.
 - [20] M. Randić, On characterization of molecular branching, *J. Am. Chem. Soc.* **97** (1975) 6609–6615.
 - [21] L. Shi, Bounds on Randić indices, *Discr. Math.* **309** (2009) 5238–5241.
 - [22] A. J. Schwenk, Computing the characteristic polynomial of a graph, in: R. Bary, F. Harary (Eds.), *Graphs and Combinatorics*, Springer-Verlag, Berlin, 1974, pp. 153–172.
 - [23] F. Zhang, *Matrix Theory – Basic Results and Techniques*, Springer, New York, 2011.