Iranian Journal of Mathematical Chemistry

IJMC

DOI: 10.22052/IJMC.2025.256371.1984
Vol. 17, No. 1, 2026, pp. 13-33
Research Paper

Properties of Laplacian Eigenvalues of Some Bicyclic and Tricyclic Graphs

Mohammad Tariq Rahim[1*], Muhammad Adnan Atta[1], Afeefa Maryam[1] and Fawad Hussain[1]

[1]Department of Mathematics, Abbottabad University of Science & Technology, Havelian, KPK, Pakistan

Keywords:
Molecular graphs,
$\pi-$electron energy,
Complement of a graph

AMS Subject Classification (2020):
05C50; 05C90

Article History:
Received: 9 March 2025
Accepted: 17 November 2025

Abstract

The Laplacian energy (LE) and the Laplacian energy-like (LEL) have recently been proposed based on molecular graph analogues of the total π-electron energy E. Both energies have been widely studied recently because of their wide range of applications. In the present work, exact expressions of the Laplacian energy and the Laplacian-like invariants of bicyclic and tricyclic molecular graphs in terms of their orders have been obtained. We also compute these expressions for the complements of these classes of graphs. It is shown that LEL is strictly less than LE for these classes of molecular graphs, but for their complements the inequality is the opposite.

1 Introduction

The energy E of the total π-electron within a conjugated system is calculated using he Hückel molecular orbital (HMO) model, and is one of the classical approaches to studying the quantum-chemical characteristics of large-size polycyclic conjugated hydrocarbons. Details and applications about this theory can be found in the literature [1–4]. In the HMO model of conjugated π-electron systems, quantities such as the total π-electron energy E are derived from the eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ of the associated molecular graph [5, 6]. Specifically, for conjugated hydrocarbons, these eigenvalues represent the orbital energy levels determined by the graph structure:

$$E = \sum_{i=1}^{n} |\lambda_i|, \tag{1}$$

where E is measured in units of the HMO carbon-carbon resonance parameter β.
Equation (1) provides a basis for defining the graph energy. In the HMO model, while E can

*Corresponding author
E-mail addresses: tariqsms@gmail.com (M. Tariq Rahim), madnan124@gmail.com (M. A. Atta), afifamalik0640@gmail.com (A. Maryam), fawadhussain998@hotmail.com (F. Hussain)
Academic Editor: Gholam Hossein Fath-Tabar

be expressed only in terms of a constrained category of molecular graphs [6], the right-hand side of Equation (1) is a thoroughly-explained parameter for all graphs. In this sense, graph energy, E, is defined as the sum of all absolute eigenvalues of the graph. This variation in the interpretation of Equatin (1) led to significant progress in the study of total π-electron energy; for further details see [7, 8].
We note that the eigenvalues $\lambda_1, \lambda_2, ..., \lambda_n$ are just the eigenvalues of the adjacency matrix. The *adjacency matrix* $\mathcal{A}(G)$ of a graph G is the 01-matrix with rows and columns indexed by the vertices of G, such that the xy-entry of $\mathcal{A}(G)$ is 1 if and only if x and y are adjacent and 0 otherwise. The eigenvalues of numerous other matrices have also been studied in graph spectral theory, in which the Laplacian matrix has gained the highest consideration in chemistry and mathematics [9]. In view of this, another invariant called the Laplacian Energy, denoted by LE(G), has been considered [10] and defined as:

$$\mathcal{LE}(G) = \sum_{i=1}^{n} \left| \mu_i - \frac{2m}{n} \right|, \tag{2}$$

where μ_i, $i = 1, 2, ..., n$ are the Laplacian eigenvalues, m represents the number of edges, and n denotes the number of vertices in the underlying graph. The right-hand sides of both Equations (1) and (2) are different. However, both can be interpreted as specific realizations of the general expression:

$$\sum_{i=1}^{n} |w_i - \bar{w}|, \tag{3}$$

where $\bar{w}$ represents the mean of the eigenvalues of $w_1, w_2, ..., w_n$.
It has been proven that several properties of LE coincide with those of E [10–13], whereas in some others, both energies (LE and E) are considerably different. However, no general results have been reported that establish the relationship between the two energies. It is well established that the key parameters determining the total energy of π-electrons are n (= the number of C atoms, i.e., the number of vertices of the molecular graph) and m (= the number of C-C bonds, i.e., the number of edges of the underlying molecular graph) [1, 3].

1.1 LE and LEL

The concept of LE entails two fundamental disadvantages, as follows: neither does $\mathcal{LE}(G_1 \cup G_2) = \mathcal{LE}(G_1) + \mathcal{LE}(G_2)$ holds in the general case, $G_1 \cup G_2$ being the molecular graph depending on two disconnected components G_1 and G_2, nor does the expression $\mathcal{LE}(G \cup K_1) = \mathcal{LE}(G)$ holds, where K_1 is the molecular graph with one vertex. To address these difficulties, J. Liu and B. Liu developed the LEL *invariant* (or simply referred to as LEL) $\mathcal{LEL}(G)$, defined as[14].

$$\mathcal{LEL}(G) = \sum_{i=1}^{n} \sqrt{\mu_i}. \tag{4}$$

For its basic properties, see[14–16]. Interestingly, the relations $\mathcal{LEL}(G_1 \cup G_2) = \mathcal{LEL}(G_1) + \mathcal{LEL}(G_2)$ and $\mathcal{LE}(G \cup K_1) = \mathcal{LE}(G)$ hold.
Now, for clarity, we focus on the following classes of bicyclic and tricyclic molecular graphs as shown in Figure 1. Here, $p, q, r, s, t \geq 1$ represent pendent vertices in the corresponding molecular graph. The order of $\mathfrak{B}_n(p)$ is $n = p + 5$, the order of $\mathfrak{B}_n(q)$ is $q + 4 = n$, the order of $\mathfrak{t}_n(r)$ is $r + 7 = n$, the order of $\mathfrak{t}_n(s)$ is $s + 6 = n$, the order of $\mathfrak{t}_n(t)$ is $t + 5 = n$ and the order of $\mathfrak{t}_n(w)$ is $w + 4 = n$.

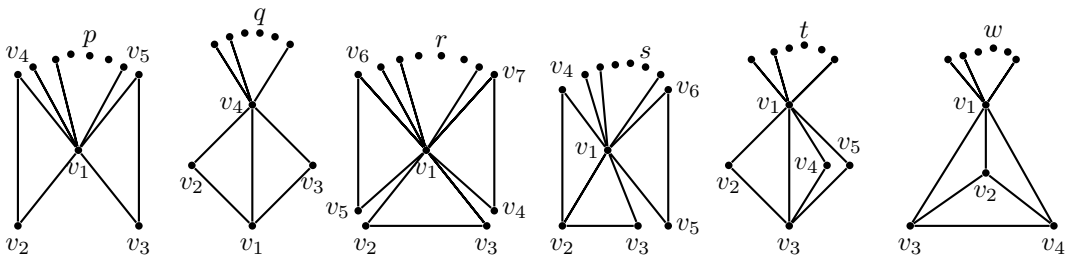

Figure 1: The graphs $\mathfrak{B}_n(p)$, $\mathfrak{B}_n(q)$, $\mathfrak{t}_n(r)$, $\mathfrak{t}_n(s)$, $\mathfrak{t}_n(t)$, $\mathfrak{t}_n(w)$, respectively.

In this paper, we give exact expressions for LE and LEL of the above molecular graphs along with their complements. Further, we show that LE is strictly greater than LEL for every class of the above molecular graphs, but for their complements the inequality is opposite.
The paper is organized as follows: In Section 2, we give some known definitions and results. In Section 3, we calculate the Laplacian energy and Laplacian-energy-like of bicyclic molecular graphs with exactly 2 and 3 cycles, and show how LE and LEL are related for these classes of graphs. In Section 4, we calculate the Laplacian energy and Laplacian-energy-like of tricyclic molecular graphs and establish the relationship between LE and LEL for these molecular graphs. A brief conclusion is provided in Section 5.

2 Definitions and known results

In this work, only finite, simple, and undirected molecular graphs are taken into account. A *molecular graph* G is formally described by two fundamental components: the vertex set $V(G)$ and the edge set $\mathcal{E}(G)$. The *order* of G refers to the total number of vertices it contains, which is usually denoted by $n = |V(G)|$, while the *size* of G indicates the total number of its edges, written as $m = |\mathcal{E}(G)|$. For a vertex $v \in V(G)$, the *degree* $d(v)$ is defined as the number of edges incident with v. A vertex with degree one is called a *pendent vertex*, as it is connected to the graph through a single edge only. In the study of molecular graphs, pendent vertices often play a crucial role since they represent atoms that are bonded to the rest of the molecule at just one point.
Let G be a connected molecular graph with n vertices and m edges. The graph G is referred to as *k-cyclic* whenever the relation $m = n - 1 + k$ holds. In the special case $k = 0$, G corresponds to a tree, that is, an acyclic molecular graph. The *complement* of a molecular graph G, denoted by $\overline{G}$, is the graph constructed on the same vertex set as G, that is $V(\overline{G}) = V(G)$. In $\overline{G}$, two different vertices are considered adjacent precisely when they are not adjacent in G. The *Laplacian matrix* of a graph G is written as $\mathcal{L}(G) = D(G) - A(G)$, where $D(G)$ represents the degree matrix and $A(G)$ stands for the adjacency matrix. More explicitly, the degree matrix has the form $D(G) = \mathrm{diag}(d_1, d_2, \ldots, d_n)$, with each diagonal entry d_i corresponding to the degree of the vertex $v_i \in V(G)$.
The eigenvalues of the Laplacian matrix $\mathcal{L}(G)$ of a graph G are denoted by $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} \geq \mu_n$. These values are referred to as the *Laplacian eigenvalues* of G. It is well known that all Laplacian eigenvalues are real and nonnegative. In particular, the smallest eigenvalue is always $\mu_n = 0$, while the second–smallest, μ_{n-1}, often called the *algebraic connectivity*, satisfies

$\mu_{n-1} < 1$. Moreover, the Laplacian spectrum of G satisfies the following two basic relations:

$$\sum_{i=1}^{n} \mu_i = 2m, \tag{5}$$

$$\sum_{i=1}^{n} \mu_i^2 = 2m + \sum_{i=1}^{n} d_i^2, \tag{6}$$

where d_i denotes the degree of the vertex v_i. These spectral identities are frequently employed when computing various graph energies. They also serve as a foundation for deriving inequalities involving Laplacian eigenvalues and degree-based graph invariants.

Lemma 2.1. *([17]). If G is a molecular graph with complement $\overline{G}$, then the Laplacian matrix of $\overline{G}$ can be expressed as $\mathcal{L}(\overline{G}) = nI - J - \mathcal{L}(G)$, where I denotes the identity matrix of order n and J is the $n \times n$ matrix whose entries are all equal to 1.*

3 LE and LEL of $\mathfrak{B}_n(p)$ and $\mathfrak{B}_n(q)$

In this section, we determine the LE and LEL values for $\mathfrak{B}_n(p)$ and $\mathfrak{B}_n(q)$ and their complements. We begin with the following lemma.

Lemma 3.1. *For a bicyclic molecular graph $G \cong \mathfrak{B}_n(p)$ consisting of precisely two cycles together having p pendent vertices, the following hold:*
(1) *The count of edges in G is $m = n + 1$,*
(2) *The count of edges in $\overline{G}$ is $m = \frac{n^2-3n-2}{2}$.*

Theorem 3.2. *For a bicyclic molecular graph $G \cong \mathfrak{B}_n(p)$ with precisely two cycles and p pendent vertices of order $n = p + 5$, the following are true:*
(1) $\mathcal{LE}(G) = \frac{2}{n}(n^2 - 2n - 6)$,
(2) $\mathcal{LE}(\overline{G}) = \frac{3}{n}(n^2 - 3n - 2)$.

Proof. (1): First, we give the Laplacian matrix of G, (see figure of $\mathfrak{B}_n(p)$ in subsection 1.1).

$$\mathcal{L}(G) = \begin{bmatrix} n-1 & -1 & -1 & -1 & -1 & -1 & \cdots & -1 \\ -1 & 2 & -1 & 0 & 0 & 0 & \cdots & 0 \\ -1 & -1 & 2 & 0 & 0 & 0 & \cdots & 0 \\ -1 & 0 & 0 & 2 & -1 & 0 & \cdots & 0 \\ -1 & 0 & 0 & -1 & 2 & 0 & \cdots & 0 \\ -1 & 0 & 0 & 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & 0 & 0 & 0 & 0 & 0 & \cdots & 1 \end{bmatrix},$$

denote by $\chi(\mathcal{L}(G))$, the characteristic polynomial of $\mathcal{L}(G)$, by using the definition $\chi(\mu) = |\mathcal{L}(G) - \mu I|$, we get the following characteristic polynomial of $\mathcal{L}(G)$:

$$\chi(\mathcal{L}(G)) = \mu(\mu - n)(\mu - 3)^2(\mu - 1)^{n-4}. \tag{7}$$

Clearly, 0, n, 3 and 1 are zeros of the equation $\chi(\mathcal{L}(G)) = 0$, and hence are the Laplacian eigenvalues of $\mathcal{L}(G)$ with multiplicities 1, 1, 2 and $n-4$ respectively. Since Equation (7) defines

the characteristic polynomial of $\mathcal{L}(G)$. We will use Equation (2) to calculate the Laplacian energy of G.

$$\mathcal{LE}(G) = \left|0 - \frac{2n+2}{n}\right| + \left|n - \frac{2n+2}{n}\right| + 2\left|3 - \frac{2n+2}{n}\right| + (n-4)\left|1 - \frac{2n+2}{n}\right|, \tag{8}$$

since, $n \geq 6$ as $p \geq 1$, this implies that $\left|n - \frac{2n+2}{n}\right| > 0$. Now, Equation (8) takes the following form

$$\begin{aligned}\mathcal{LE}(G) &= \frac{2n+2}{n} + \frac{n^2-2n-2}{n} + 2(\frac{n-2}{n}) + (n-4)(\frac{n+2}{n}) \\ &= \frac{2}{n}(n^2-2n-6).\end{aligned} \tag{9}$$

(2): First, we give the Laplacian matrix of $\overline{G}$.

$$\mathcal{L}(\overline{G}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & n-3 & 0 & -1 & -1 & -1 & \cdots & -1 \\ 0 & 0 & n-3 & 0 & -1 & -1 & \cdots & -1 \\ 0 & -1 & -1 & n-3 & 0 & -1 & \cdots & -1 \\ 0 & -1 & -1 & -1 & n-3 & -1 & \cdots & -1 \\ 0 & -1 & -1 & -1 & -1 & n-2 & \cdots & -1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & -1 & -1 & -1 & -1 & -1 & \cdots & n-2 \end{bmatrix},$$

denote by $\chi(\mathcal{L}(\overline{G}))$, the characteristic polynomial of $\mathcal{L}(\overline{G})$, by using the definition $\chi(\mathcal{L}(\overline{G})) =| \mathcal{L}(\overline{G}) - \mu I \,|$, we get the following characteristic polynomials of $\mathcal{L}(\overline{G})$:

$$\chi(\mathcal{L}(\overline{G})) = \begin{cases} \mu^2(\mu-n+3)^2(\mu-n+1)^{n-4}, & \text{if } n \text{ is even} \\ -\mu^2(\mu-n+3)^2(\mu-n+1)^{n-4}, & \text{if } n \text{ is odd.} \end{cases}$$

Clearly, 0, $n-3$ and $n-1$ are the zeros of the equation $\chi(\mathcal{L}(\overline{G})) = 0$, and hence are the Laplacian eigenvalues of $\mathcal{L}(\overline{G})$ with multiplicities 2, 2 and $n-4$, respectively. Now, we use Equation (2) to calculate the Laplacian energy of $\overline{G}$.

$$\begin{aligned}\mathcal{LE}(\overline{G}) &= \left|0 - \frac{n^2-3n-2}{n}\right| + 2\left|(n-3) - \frac{n^2-3n-2}{n}\right| + (n-4)\left|(n-1) - \frac{n^2-3n-2}{n}\right| \\ &= \frac{n^2-3n-2}{n} + \frac{4}{n} + (n-4)\left(\frac{2n+2}{n}\right) \\ &= \frac{3}{n}(n^2-3n-2).\end{aligned} \tag{10}$$

This completes the proof. ■

Below, as a corollary, we give the LEL of $\mathfrak{B}_n(p)$ and of the complement of $\mathfrak{B}_n(p)$.

Corollary 3.3. *Consider a bicyclic molecular graph $G \cong \mathfrak{B}_n(p)$ with two cycles and p pendent vertices of order $n = p+5$. The following assertions are valid:*
(1) $\mathcal{LEL}(G) = \sqrt{n} + 2\sqrt{3} + (n-4)$,
(2) $\mathcal{LEL}(\overline{G}) = 2\sqrt{n-3} + (n-4)\sqrt{(n-1)}$.

Proof. By Theorem 3.2, the Laplacian eigenvalues of G are 0, n, 3 and 1 with multiplicities 1, 1, 2 and $n-4$, respectively. Also 0, $n-3$ and $n-1$ are the Laplacian eigenvalues of $\overline{G}$ with multiplicities 2, 2 and $n-4$ respectively. Now, by using Equation (4) the result follows. ■

Now, we discuss the LE and LEL of the bicyclic molecular graph with exactly three cycles, i.e., of $\mathfrak{B}_n(q)$ (for the figure of $\mathfrak{B}_n(q)$ see subsection 1.1). Note that the graph $\mathfrak{B}_n(q)$ has order $n = q+4$ for $q \geq 1$ (an integer) pendent vertices. First, we give the following lemma.

Lemma 3.4. *Let $G \cong \mathfrak{B}_n(q)$ be a bicyclic molecular graph consisting of precisely three cycles together with q pendant vertices. For this graph, the following are valid:*
(1) *The count of edges in G is $m = n+1$,*
(2) *The count of edges in $\overline{G}$ is $m = \frac{n^2-3n-2}{2}$.*

Proof. (1) and (2) hold by Lemma 3.1. ■

Theorem 3.5. *Consider a bicyclic molecular graph $G \cong \mathfrak{B}_n(p)$ with three cycles and q pendent vertices, having order $n = q+4$. The following must follow:*
(1) $\mathcal{LE}(G) = \frac{1}{4}(2n-4)(n+2)$,
(2) $\mathcal{LE}(\overline{G}) = \frac{1}{n}(4n^2-10n+8)$.

Proof. (1): First, we give the Laplacian matrix of G, (see figure of $\mathfrak{B}_n(q)$ in subsection 1.1) as:

$$\mathcal{L}(G) = \begin{bmatrix} 3 & -1 & -1 & -1 & 0 & 0 & \cdots & 0 \\ -1 & 2 & 0 & -1 & 0 & 0 & \cdots & 0 \\ -1 & 0 & 2 & -1 & 0 & 0 & \cdots & 0 \\ -1 & -1 & -1 & n-1 & -1 & -1 & \cdots & -1 \\ 0 & 0 & 0 & -1 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & -1 & 0 & 0 & \cdots & 1 \end{bmatrix}.$$

Let $\chi(\mathcal{L}(G))$, denote the characteristic polynomial of $\mathcal{L}(G)$. By using the definition $\chi(\mathcal{L}(G)) = |\, \mathcal{L}(G) - \mu I \,|$, we get the following characteristic polynomials of $\mathcal{L}(G)$:

$$\chi(\mathcal{L}(G)) = \begin{cases} \mu^2(\mu-1)^{n-4}(\mu-2)(\mu-4)(\mu-n), & \text{if } n \text{ is even}, \\ -\mu^2(\mu-1)^{n-4}(\mu-2)(\mu-4)(\mu-n), & \text{if } n \text{ is odd}. \end{cases}$$

Clearly, 0, 1, 2, 4 and n are the roots of the equation $\chi(\mathcal{L}(G)) = 0$, and hence are the Laplacian eigenvalues of $\mathcal{L}(G)$ with multiplicities 2, $n-4$, 1, 1 and 1, respectively. We then use Equation (2) to calculate the Laplacian energy of G:

$$\mathcal{LE}(G) = \left|0 - \frac{2n+2}{n}\right| + (n-4)\left|1 - \frac{2n+2}{n}\right| + \left|2 - \frac{2n+2}{n}\right| + \left|4 - \frac{2n+2}{n}\right| + \left|n - \frac{2n+2}{n}\right|, \quad (11)$$

since, $n \geq 5$ as $q \geq 1$, this implies that $\left|4 - \frac{2n+2}{n}\right| = \frac{2n-2}{2} > 0$ and $\left|n - \frac{2n+2}{n}\right| = \frac{n^2-2n-2}{2} > 0$. Now, Equation (11) takes the following form:

$$\begin{aligned} \mathcal{LE}(G) &= \frac{2n+2}{n} + (n-4)\frac{n+2}{n} + \frac{2n-2}{n} + \frac{n^2-2n-2}{n} \\ &= \frac{(2n-4)(n+2)}{4}. \end{aligned} \quad (12)$$

(2): First, we give the Laplacian matrix of $\overline{G}$.

$$\mathcal{L}(\overline{G}) = \begin{bmatrix} n-4 & 0 & 0 & 0 & -1 & -1 & \cdots & -1 \\ 0 & n-3 & -1 & 0 & -1 & -1 & \cdots & -1 \\ 0 & -1 & n-3 & 0 & -1 & -1 & \cdots & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ -1 & -1 & -1 & 0 & n-2 & -1 & \cdots & -1 \\ -1 & -1 & -1 & 0 & -1 & n-2 & \cdots & -1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & -1 & 0 & -1 & -1 & \cdots & n-2 \end{bmatrix}.$$

Let $\chi(\mathcal{L}(\overline{G}))$, denote the characteristic polynomial of $\mathcal{L}(\overline{G})$. By using the definition $\chi(\mathcal{L}(\overline{G})) = |\mathcal{L}(\overline{G}) - \mu I|$, we get the following characteristic polynomials of $\mathcal{L}(\overline{G})$:

$$\chi(\mathcal{L}(\overline{G})) = \begin{cases} \mu^2(\mu-n+1)^{n-4}(\mu-n+4)(\mu-n+2), & \text{if } n \text{ is even}, \\ -\mu^2(\mu-n+1)^{n-4}(\mu-n+4)(\mu-n+2), & \text{if } n \text{ is odd}. \end{cases}$$

Clearly, 0, $n-2$, $n-4$ and $n-1$ are the roots of the equation $\chi(\mathcal{L}(\overline{G})) = 0$, and hence are the Laplacian eigenvalues of $\mathcal{L}(\overline{G})$ with multiplicities 2, 1, 1 and $n-4$, respectively. Now, we use Equation (2) to calculate the Laplacian energy of $\overline{G}$:

$$\begin{aligned} \mathcal{LE}(\overline{G}) &= 2\left|0 - \frac{n^2-3n-2}{n}\right| + (n-4)\left|(n-1) - \frac{n^2-3n-2}{n}\right| + \left|(n-4) - \frac{n^2-3n-2}{n}\right| \\ &\quad + \left|(n-2) - \frac{n^2-3n-2}{n}\right| \\ &= \frac{n^2-3n-2}{n} + \frac{(n-4)(2n+2)}{n} + \frac{n+2}{n} + \frac{n-2}{n} \\ &= \frac{1}{n}(4n^2-10n-8). \end{aligned} \tag{13}$$

This completes the proof. ■

Below, we give the LEL of $\mathfrak{B}_n(q)$ and of the complement of $\mathfrak{B}_n(q)$.

Corollary 3.6. *Let $G \cong \mathfrak{B}_n(q)$ be a bicyclic molecular graph consisting of precisely three cycles and q pendent vertices of order $n = q+4$. Then the following hold:*
(1) $\mathcal{LEL}(G) = (n-2) + \sqrt{n} + \sqrt{2}$,
(2) $\mathcal{LEL}(\overline{G}) = (n-4)\sqrt{n-1} + \sqrt{n-4}\sqrt{(n-2)}$.

Proof. By Theorem 3.5, the Laplacian eigenvalues of G are 0, 2, 4, n and 1 with multiplicities 2, $n-4$, 1, 1 and 1, respectively. And 0, $n-2$, $n-4$ and $n-1$ are the Laplacian eigenvalues of $\overline{G}$ with multiplicities 2, 1, 1 and $n-4$, respectively. Now, using Equation (4) the result follows. ■

3.1 *LE* versus *LEL* of $\mathfrak{B}_n(p)$, $\overline{\mathfrak{B}_n(p)}$, $\mathfrak{B}_n(q)$ and $\overline{\mathfrak{B}_n(q)}$

This section provides a graphical interpretation of the LE and LEL of the bicyclic molecular graphs, i.e., of $\mathfrak{B}_n(p)$, $\mathfrak{B}_n(q)$ and of their complements, i.e., of $\overline{\mathfrak{B}_n(q)}$, $\overline{\mathfrak{B}_n(p)}$. The main purpose of this section is to indicate the minimal and maximal LE and this part of the paper is designed

to LEL of the aforementioned molecular graphs with 2000000 vertices, for this we have used Python. The orange line in the graphs indicates LEL, and the blue line indicates LE in the aforementioned molecular graphs. We have plotted LE and LEL along the x-axis and the number of vertices along the y-axis.
From Figures 2 and 4, we observe that initially LE and LEL coincide, but when the number of vertices increases, then LE increases for $\mathfrak{B}_n(p)$ and $\mathfrak{B}_n(q)$. On the other hand, we face the opposite situation, i.e., in Figures 3 and 5, we see that initially the LE and LEL coincide, but when the order increases, then LE decreases for $\overline{\mathfrak{B}_n(p)}$ and $\overline{\mathfrak{B}_n(q)}$.

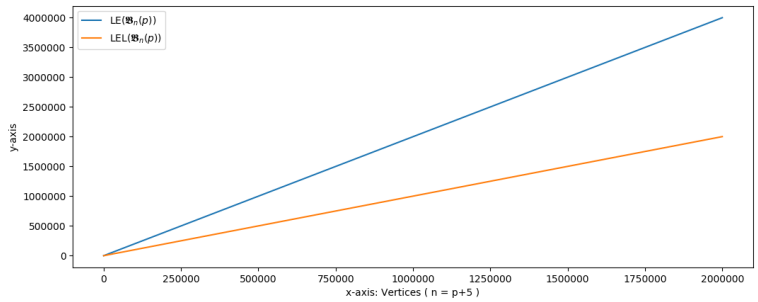

Figure 2: The LE versus LEL of the bicyclic molecular graph $\mathfrak{B}_n(p)$. The data set consists of the LE and LEL of $\mathfrak{B}_n(p)$ with n vertices, where $6 \leq n \leq 2000000$. Clearly, the data set shows that LEL is strictly less than LE for $\mathfrak{B}_n(p)$ up to 2000000 number of vertices.

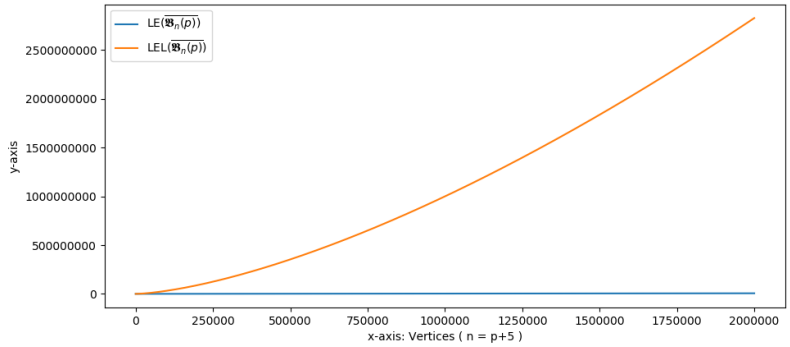

Figure 3: The LE versus LEL of the bicyclic molecular graph $\overline{\mathfrak{B}_n(p)}$. The data set consists of the LE and LEL of $\overline{\mathfrak{B}_n(p)}$ with n vertices, where $6 \leq n \leq 2000000$. Clearly, the data set shows that LE is strictly less than LEL for $\overline{\mathfrak{B}_n(p)}$ up to 2000000 number of vertices.

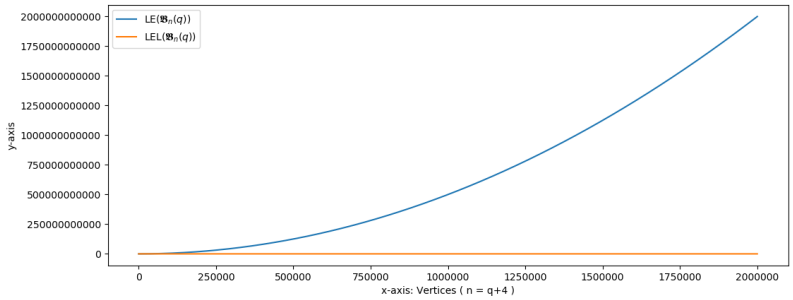

Figure 4: The LE versus LEL of the bicyclic molecular graph $\mathfrak{B}_n(q)$. The data set consists of the LE and LEL of $\mathfrak{B}_n(q)$ with n vertices, where $5 \leq n \leq 2000000$. Clearly, the data set shows that LEL is strictly less than LE for $\mathfrak{B}_n(q)$ up to 2000000 number of vertices.

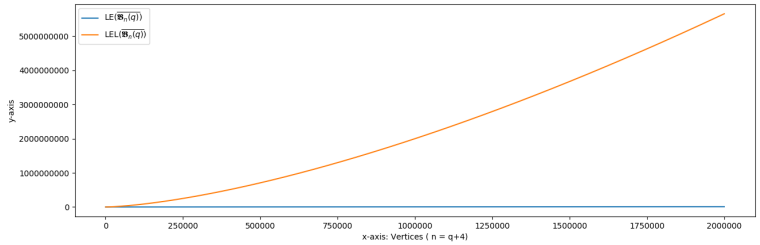

Figure 5: The LE versus LEL of the bicyclic molecular graph $\overline{\mathfrak{B}_n(q)}$. The data set consists of the LE and LEL of $\overline{\mathfrak{B}_n(q)}$ with n vertices, where $5 \leq n \leq 2000000$. Clearly, the data set shows that LE is strictly less than LEL of $\overline{\mathfrak{B}_n(q)}$ up to 2000000 number of vertices.

4 LE and LEL of $\mathfrak{t}_n(r)$, $\mathfrak{t}_n(s)$, $\mathfrak{t}_n(t)$ and $\mathfrak{t}_n(w)$

In this section, we find the Laplacian energy and Laplacian-energy-like for some families of tricyclic molecular graphs as shown in Subsection 1.1.

Lemma 4.1. *Suppose $G \cong \mathfrak{t}_n(r)$ is a tricyclic molecular graph that contains precisely three cycles and r pendent vertices. We have:*
(1) *The number of edges in G is $m = n + 2$,*
(2) *The number of edges in $\overline{G}$ is $m = \frac{n^2-3n-4}{2}$.*

Proof. (1) and (2) hold by Lemma 3.1. ■

Remark 1. It is not hard to see that $\mathfrak{t}_n(s)$, $\mathfrak{t}_n(t)$ and $\mathfrak{t}_n(w)$ have $m = n + 2$ edges, and their complements have $m = \frac{n^2-3n-4}{2}$ edges.

Theorem 4.2. *Suppose that $G \cong \mathfrak{t}_n(r)$ is a tricyclic molecular graph that contains precisely three cycles together with r pendent vertices of order $n = r + 7$. Then, the following assertions are valid:*
(1) $\mathcal{LE}(G) = \frac{2}{n}(n^2 + n - 16)$,
(2) $\mathcal{LE}(\overline{G}) = \frac{4}{n}(n^2 - 3n - 4)$.

Proof. (1): First, we give the Laplacian matrix of G, (see figure of $\mathfrak{t}_n(r)$ in Subsection 1.1).

$$\mathcal{L}(G) = \begin{bmatrix} n-1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & \cdots & -1 \\ -1 & 2 & -1 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ -1 & -1 & 2 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ -1 & 0 & 0 & 2 & -1 & 0 & 0 & 0 & \cdots & 0 \\ -1 & 0 & 0 & -1 & 2 & 0 & 0 & 0 & \cdots & 0 \\ -1 & 0 & 0 & 0 & 0 & 2 & -1 & 0 & \cdots & 0 \\ -1 & 0 & 0 & 0 & 0 & -1 & 2 & 0 & \cdots & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 1 \end{bmatrix}.$$

Let $\chi(\mathcal{L}(G))$ denote the characteristic polynomial of $\mathcal{L}(G)$. Then, we get the following characteristic polynomial of $\mathcal{L}(G)$:

$$\chi(\mathcal{L}(G)) = \mu(\mu - n)(\mu - 3)^3(\mu - 1)^{n-5}. \tag{14}$$

Clearly, 0, n, 3 and 1 are the roots of the equation $\chi(\mathcal{L}(G)) = 0$, and hence 0,n, 3 and 1 are the Laplacian eigenvalues of $\mathcal{L}(G)$ with multiplicities 1, 1, 3 and $n-5$ respectively. Note that, one can verify that the polynomial (14) is the characteristic polynomial of $\mathcal{L}(G)$ by using Equation (5) and Lemma 4.1 (1). Now, we use Equation (2) to calculate the Laplacian energy of G.

$$\mathcal{LE}(G) = \left|0 - \frac{2n+4}{n}\right| + \left|n - \frac{2n+4}{n}\right| + 3\left|3 - \frac{2n+4}{n}\right| + (n-5)\left|1 - \frac{2n+4}{n}\right|, \tag{15}$$

since, $n \geq 8$ as $p \geq 1$, this implies that $\left|n - \frac{2n+4}{n}\right| > 0$. Now, Equation (15) takes the following form:

$$\begin{aligned} \mathcal{LE}(G) &= \frac{2n+4}{n} + \frac{n^2-2n-4}{n} + 3\left(\frac{n-4}{n}\right) + (n-5)\left(\frac{n+4}{n}\right) \\ &= \frac{2}{n}(n^2+n-16). \end{aligned} \tag{16}$$

(2): First, we give the Laplacian matrix of $\overline{G}$, (see figure of $\mathfrak{t}_n(r)$ in Subsection 1.1):

$$\mathcal{L}(\overline{G}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & n-3 & -1 & -1 & -1 & -1 & -1 & \cdots & -1 & \\ 0 & 0 & n-3 & -1 & -1 & -1 & -1 & -1 & \cdots & -1 \\ 0 & -1 & -1 & n-3 & -1 & -1 & -1 & -1 & \cdots & -1 \\ 0 & -1 & -1 & 0 & n-3 & -1 & -1 & -1 & \cdots & -1 \\ 0 & -1 & -1 & -1 & -1 & n-3 & 0 & -1 & \cdots & -1 \\ 0 & -1 & -1 & -1 & -1 & 0 & n-3 & -1 & \cdots & -1 \\ 0 & -1 & -1 & -1 & -1 & -1 & -1 & n-2 & \cdots & -1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & \cdots & n-2 \end{bmatrix}.$$

If $\chi(\mathcal{L}(\overline{G}))$ denote the characteristic polynomial of $\mathcal{L}(\overline{G})$. Then, we get the following characteristic polynomials of $\mathcal{L}(\overline{G})$:

$$\chi(\mathcal{L}(\overline{G})) = \mu^2(\mu - (n-3))^3(\mu - (n-1))^{n-5}. \tag{17}$$

Clearly, 0, $n-3$ and $n-1$ are the zeros of $\chi(\mathcal{L}(\overline{G}))=0$, and hence 0, $n-3$ and $n-1$ are the Laplacian eigenvalues of $\mathcal{L}(\overline{G})$ with multiplicities 2, 3 and $n-5$ respectively. Now, we use Equation (2) to calculate the Laplacian energy of $\overline{G}$.

$$\begin{aligned}\mathcal{LE}(\overline{G}) &= \left|0-\frac{n^2-3n-4}{n}\right|+3\left|(n-3)-\frac{n^2-3n-4}{n}\right|+(n-5)\left|(n-1)-\frac{n^2-3n-4}{n}\right| \\ &= \frac{2n^2-3n-4}{n}+\frac{12}{n}+(n-5)\left(\frac{2n+4}{n}\right) \\ &= \frac{4}{n}(n^2-3n-4).\end{aligned} \tag{18}$$

■

Below, as a corollary, we give the Laplacian-energy-like of $\mathfrak{t}_n(r)$ and of its complement.

Corollary 4.3. *Let $G\cong\mathfrak{t}_n(r)$ be a tricyclic molecular graph that contains precisely three cycles and r pendent vertices of order $n=r+7$. Then:*
(1) $\mathcal{LEL}(G)=\sqrt{n}+3\sqrt{3}+(n-5)$,
(2) $\mathcal{LEL}(\overline{G})=3\sqrt{n-3}+(n-5)\sqrt{(n-1)}$.

Proof. Because, by Theorem 4.2, we have that 0, n, 3 and 1 are the Laplacian eigenvalues of G with multiplicities 1, 1, 3 and $n-5$ respectively. And 0, $n-3$ and $n-1$ are the Laplacian eigenvalues of $\overline{G}$ with multiplicities 2, 3 and $n-5$ respectively. Now, using Equation (4) the result follows. ■

Theorem 4.4. *Let $G\cong\mathfrak{t}_n(s)$ be a tricyclic molecular graph that contains precisely four cycles together with s pendent vertices of order $n=s+6$. The following statements are valid:*
(1) $\mathcal{LE}(G)=\frac{2}{n}(n^2+n-12)$,
(2) $\mathcal{LE}(\overline{G})=\frac{2}{n}(2n^2-5n-12)$.

Proof. First, we give the Laplacian matrix of G, (see figure of $\mathfrak{t}_n(s)$ in Subsection 1.1).

$$\mathcal{L}(G)=\begin{bmatrix} n-1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & \cdots & -1 \\ -1 & 2 & -1 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ -1 & -1 & 2 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ -1 & 0 & 0 & 2 & 0 & -1 & 0 & 0 & \cdots & 0 \\ -1 & 0 & 0 & 0 & 2 & -1 & 0 & 0 & \cdots & 0 \\ -1 & 0 & 0 & -1 & -1 & 3 & 0 & 0 & \cdots & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 1 \end{bmatrix}.$$

Let $\chi(\mathcal{L}(G))$ denote the characteristic polynomial of $\mathcal{L}(G)$. Using the definition $\chi(\mathcal{L}(G))=|\mathcal{L}(G)-\mu I|$, we get the following characteristic polynomials of $\mathcal{L}(G)$:

$$\chi(\mathcal{L}(G))=\mu(\mu-1)^{n-5}(\mu-2)(\mu-3)(\mu-4)(\mu-n). \tag{19}$$

Clearly, 0, 1, 2,3, 4 and n are the roots of the equation $\chi(\mathcal{L}(G))=0$, and hence 0, 1, 2,3, 4 and n are the Laplacian eigenvalues of $\mathcal{L}(G)$ with multiplicities 1, $n-5$,1, 1, 1 and 1 respectively.

Now, we use Equation (2) to calculate the Laplacian energy of G:

$$\begin{aligned}\mathcal{LE}(G) &= \left|0-\frac{2n+4}{n}\right| + (n-5)\left|1-\frac{2n+4}{n}\right| + \left|2-\frac{2n+4}{n}\right| + \left|3-\frac{2n+4}{n}\right| + \left|4-\frac{2n+4}{n}\right| \\ &+ \left|n-\frac{2n+4}{n}\right| = \frac{2n+4}{n} + (n-5)\frac{n+4}{n} + \frac{4}{n} + \frac{n-4}{n} + \frac{2n-4}{n} + \frac{n^2-2n-4}{n} \\ &= \frac{2}{n}(n^2+n-12).\end{aligned} \tag{20}$$

(2): First, we give the Laplacian matrix of $\overline{G}$, (see figure of $\mathfrak{t}_n(s)$ in Subsection 1.1):

$$\mathcal{L}(\overline{G}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & n-3 & 0 & -1 & -1 & -1 & -1 & -1 & \cdots & -1 \\ 0 & 0 & n-3 & -1 & -1 & -1 & -1 & -1 & \cdots & -1 \\ 0 & -1 & -1 & n-3 & -1 & -1 & -1 & -1 & \cdots & -1 \\ 0 & -1 & -1 & -1 & n-3 & -1 & -1 & -1 & \cdots & -1 \\ 0 & -1 & -1 & 0 & 0 & n-4 & -1 & -1 & \cdots & -1 \\ 0 & -1 & -1 & -1 & -1 & -1 & n-2 & -1 & \cdots & -1 \\ 0 & -1 & -1 & -1 & -1 & -1 & -1 & n-2 & \cdots & -1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & \cdots & n-2 \end{bmatrix}.$$

Let $\chi(\mathcal{L}(\overline{G}))$, denote the characteristic polynomial of $\mathcal{L}(\overline{G})$. Then, we get the following characteristic polynomials of $\mathcal{L}(\overline{G})$:

$$\chi(L(\bar{G})) = \mu^2(\mu-(n-4))(\mu-(n-3))(\mu-(n-2))(\mu-(n-1))^{n-5}. \tag{21}$$

Clearly, 0, $n-4$, $n-3$, $n-2$ and $n-1$ are the roots of the equation $\chi(\mathcal{L}(\overline{G}) = 0$, and hence 0, $n-4$, $n-3$, $n-2$ and $n-1$ are the Laplacian eigenvalues of $\mathcal{L}(\overline{G})$ with multiplicities 2, 1, 1,1 and $n-5$, respectively. Now, we use Equation (2) to calculate the Laplacian energy of G.

$$\begin{aligned}\mathcal{LE}(\overline{G}) &= 2\left|0-\frac{n^2-3n-4}{n}\right| + \left|(n-4)-\frac{n^2-3n-4}{n}\right| + \left|(n-3)-\frac{n^2-3n-4}{n}\right| + \\ &\left|(n-2)-\frac{n^2-3n-4}{n}+\right| (n-5)\left|(n-1)-\frac{n^2-3n-4}{n}\right| \\ &= \frac{2(n^2-3n-2)}{n} + \frac{n-4}{n} + \frac{4}{n} + \frac{n+4}{n} + (n-5)\left(\frac{2n+4}{n}\right) \\ &= \frac{2}{n}(2n^2-5n-12).\end{aligned} \tag{22}$$

■

Corollary 4.5. *Let $G \cong \mathfrak{t}_n(s)$ be a tricyclic molecular graph that contains precisely four cycles and s pendent vertices of order $n = s+6$. Then the following hold:*
(1) $\mathcal{LEL}(G) = \sqrt{n}+n+\sqrt{3}+\sqrt{2}-3$,
(2) $\mathcal{LEL}(\overline{G}) = \sqrt{n-3}+\sqrt{n-4}+\sqrt{n-2}+(n-5)\sqrt{n-1}$.

Proof. Because, by Theorem 4.4, we have that 0,1,2,3,4 and n are the Laplacian eigenvalues of G with multiplicities 1, $n-5$, 2,3,4 and n, respectively. And 0, $n-4$,$n-3$, $n-2$ and $n-1$ are the Laplacian eigenvalues of $\overline{G}$ with multiplicities 2, 1,1,1 and $n-5$ respectively. Now, using Equation (4) the result follows. ■

Theorem 4.6. *Let $G \cong \mathfrak{t}_n(t)$ be a tricyclic molecular graph that contains precisely six cycles together with t pendent vertices of order $n = t + 5$. Then, the following hold:*
(1) $\mathcal{LE}(G) = \frac{2}{n}(n^2 + n - 8)$,
(2) $\mathcal{LE}(\overline{G}) = \frac{4}{n}(n^2 - 2n - 6)$.

Proof. (1): First, we give the Laplacian matrix of G, (see figure of $\mathfrak{t}_n(t)$ in Subsection 1.1):

$$\mathcal{L}(G) = \begin{bmatrix} n-1 & -1 & -1 & -1 & -1 & -1 & -1 & \cdots & -1 \\ -1 & 2 & 0 & 0 & -1 & 0 & 0 & \cdots & 0 \\ -1 & 0 & 2 & 0 & -1 & 0 & 0 & \cdots & 0 \\ -1 & 0 & 0 & 2 & -1 & 0 & 0 & \cdots & 0 \\ -1 & -1 & -1 & -1 & 4 & -1 & 0 & \cdots & 0 \\ -1 & 0 & 0 & 0 & 0 & 1 & 0 & \cdots & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 1 \end{bmatrix}.$$

Let $\chi(\mathcal{L}(G))$ denote the characteristic polynomial of $\mathcal{L}(G)$. We get the following characteristic polynomial of $\mathcal{L}(G)$:

$$\chi(\mathcal{L}(G)) = \mu(\mu-1)^{n-5}(\mu-2)^2(\mu-5)(\mu-n). \tag{23}$$

Clearly, 0,1,2 5 and n are the roots of the equation $\chi(\mathcal{L}(G)) = 0$, and hence 0,1,2 5 and n are the Laplacian eigenvalues of $\mathcal{L}(G)$ with multiplicities 1, $n-5$, 2,1 and 1 respectively. Now, we use Equation (2) to calculate the Laplacian energy of G:

$$\begin{aligned} \mathcal{LE}(G) &= \left|0 - \frac{2n+4}{n}\right| + (n-5)\left|1 - \frac{2n+4}{n}\right| + 2\left|2 - \frac{2n+4}{n}\right| + \left|5 - \frac{2n+4}{n}\right| + \left|n - \frac{2n+4}{n}\right| \\ &= \frac{2n+4}{n} + (n-5)\frac{n+4}{n} + \frac{2.4}{n} + \frac{3n-4}{n} + \frac{n^2-2n-4}{n} \\ &= \frac{2}{n}(n^2+n-8). \end{aligned} \tag{24}$$

(2): First, we give the Laplacian matrix of $\overline{G}$, (see figure of $\mathfrak{t}_n(t)$ in Subsection 1.1):

$$\mathcal{L}(\overline{G}) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & n-3 & -1 & -1 & 0 & -1 & -1 & \cdots & -1 \\ 0 & -1 & n-3 & -1 & 0 & -1 & -1 & \cdots & -1 \\ 0 & -1 & -1 & n-3 & 0 & -1 & -1 & \cdots & -1 \\ 0 & 0 & 0 & 0 & n-5 & -1 & -1 & \cdots & -1 \\ 0 & -1 & -1 & -1 & -1 & n-2 & -1 & \cdots & -1 \\ 0 & -1 & -1 & -1 & -1 & -1 & n-2 & \cdots & -1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & -1 & -1 & -1 & -1 & -1 & -1 & \cdots & n-2 \end{bmatrix}.$$

Let $\chi(\mathcal{L}(\overline{G}))$ denote the characteristic polynomial of $\mathcal{L}(\overline{G})$. We get the following characteristic polynomials of $\mathcal{L}(\overline{G})$:

$$\chi(\mathcal{L}(\overline{G})) = \mu^2(\mu-(n-5))(\mu-(n-2))^2(\mu-(n-1))^{n-5}. \tag{25}$$

Clearly, 0, $n-5$, $n-2$ and $n-1$ are the roots of the equation $\chi(\mathcal{L}(G))=0$, and hence 0, $n-5$, $n-2$ and $n-1$ are the Laplacian eigenvalues of $\mathcal{L}(\overline{G})$ with multiplicities 2, 1, 2 and $n-5$, respectively. Now, we use Equation (2) to calculate the Laplacian energy of G.

$$\begin{aligned}\mathcal{LE}(\overline{G}) &= 2\left|0-\frac{n^2-3n-4}{n}\right|+\left|(n-5)-\frac{n^2-3n-4}{n}\right|+\\ &\quad 2\left|(n-2)-\frac{n^2-3n-4}{n}\right|+(n-5)\left|(n-1)-\frac{n^2-3n-4}{n}\right|\\ &= \frac{2(n^2-3n-2)}{n}+\frac{2n-4}{n}+\frac{2(n+4)}{n}+(n-5)\left(\frac{2n+4}{n}\right)\\ &= \frac{4}{n}(n^2-2n-6).\end{aligned} \tag{26}$$

■

Corollary 4.7. *Let $G\cong \mathfrak{t}_n(t)$ be a tricyclic molecular graph that contains precisely six cycles together with t pendent vertices of order $n=t+5$. Then, the following hold:*
(1) $\mathcal{LEL}(G)=\sqrt{n}+n+\sqrt{5}-5+2\sqrt{2}$,
(2) $\mathcal{LEL}(\overline{G})=\sqrt{n-5}+\sqrt{n-2}+(n-5)\sqrt{n-1}$.

Proof. Because, by Theorem 4.6, we have that 0, 1, 2, 5 and n are the Laplacian eigenvalues of G with multiplicities 1, $n-5$, 2, 1 and 1, respectively. And 0, $n-5$, $n-2$ and $n-1$ are the Laplacian eigenvalues of $\overline{G}$ with multiplicities 2, 1, 2 and $n-5$, respectively. Now, by using Equation (4) the result follows. ■

Theorem 4.8. *Consider $G\cong \mathfrak{t}_n(w)$ is a tricyclic molecular graph that contains precisely seven cycles together with w pendant vertices of a given order $n=w+4$. Then, the following hold:*
(1) $\mathcal{LE}(G)=\frac{2}{n}(n^2+2n-12)$,
(2) $\mathcal{LE}(\overline{G})=\frac{4}{n}(n^2-2n-8)$.

Proof. (1): First, we give the Laplacian matrix of G, (see figure of $\mathfrak{t}_n(w)$ in Subsection 1.1):

$$\mathcal{L}(G)=\begin{bmatrix} 3 & -1 & -1 & -1 & 0 & 0 & 0 & \cdots & 0\\ -1 & 3 & -1 & -1 & 0 & 0 & 0 & \cdots & 0\\ -1 & -1 & 3 & -1 & 0 & 0 & 0 & \cdots & 0\\ -1 & -1 & -1 & n-1 & -1 & -1 & -1 & \cdots & -1\\ 0 & 0 & 0 & -1 & 1 & 0 & 0 & \cdots & 0\\ 0 & 0 & 0 & -1 & 0 & 1 & 0 & \cdots & 0\\ 0 & 0 & 0 & -1 & 0 & 0 & 1 & \cdots & 0\\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & \cdots & 1 \end{bmatrix}.$$

Let $\chi(\mathcal{L}(G))$ denote the characteristic polynomial of $\mathcal{L}(G)$. We get the following characteristic polynomial of $\mathcal{L}(G)$:

$$\chi(\mathcal{L}(G))=\mu(\mu-1)^{n-4}(\mu-4)^2(\mu-n). \tag{27}$$

Clearly, 0, 1, 4 and n are the roots of the equation $\chi(\mathcal{L}(G))=0$, and hence 0, 1, 4 and n are the Laplacian eigenvalues of $\mathcal{L}(G)$ with multiplicities 1, $n-4$, 2 and 1, respectively. Now, we

use Equation (2) to calculate the Laplacian energy of G.

$$\begin{aligned}\mathcal{LE}(G) &= \left|0-\frac{2n+4}{n}\right| + (n-4)\left|1-\frac{2n+4}{n}\right| + 2\left|4-\frac{2n+4}{n}\right| + \left|n-\frac{2n+4}{n}\right| \\ &= \frac{2n+4}{n} + (n-4)\frac{n+4}{n} + 2\frac{2n-4}{n} + \frac{n^2-2n-4}{n} \\ &= \frac{2}{n}(n^2+2n-12).\end{aligned} \tag{28}$$

(2): First, we give the Laplacian matrix of $\overline{G}$, (see figure of $\mathfrak{t}_n(w)$ in Subsection 1.1).

$$\mathcal{L}(\overline{G}) = \begin{bmatrix} n-4 & 0 & 0 & 0 & -1 & -1 & \cdots & -1 \\ 0 & n-4 & 0 & 0 & -1 & -1 & \cdots & -1 \\ 0 & 0 & n-4 & 0 & -1 & -1 & \cdots & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ -1 & -1 & -1 & 0 & n-2 & -1 & \cdots & -1 \\ -1 & -1 & -1 & 0 & -1 & n-2 & \cdots & -1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & -1 & 0 & -1 & -1 & \cdots & n-2 \end{bmatrix}.$$

Let $\chi(\mathcal{L}(\overline{G}))$ denote the characteristic polynomial of $\mathcal{L}(\overline{G})$. We get the following characteristic polynomials of $\mathcal{L}(\overline{G})$:

$$\chi(L(\overline{G})) = \mu^2(\mu-(n-4))^2(\mu-(n-1))^{n-4}. \tag{29}$$

Clearly 0, $n-4$ and $n-1$ are the zeros of $\chi(L\overline{G}) = 0$, and hence 0, $n-4$ and $n-1$ are the Laplacian eigenvalues of $L(\overline{G})$ with multiplicities 2, 2 and $n-4$, respectively. Now, we use Equation (2) to calculate the Laplacian energy of $\overline{G}$.

$$\begin{aligned}\mathcal{LE}(\overline{G}) &= 2\left|0-\frac{n^2-3n-4}{n}\right| + 2\left|(n-4)-\frac{n^2-3n-4}{n}\right| + (n-4)\left|(n-1)-\frac{n^2-3n-4}{n}\right| \\ &= \frac{2(n^2-3n-4)}{n} + \frac{2(3n)}{n} + (n-4)\left(\frac{2n+4}{n}\right) \\ &= \frac{4}{n}(n-3)(n+2).\end{aligned} \tag{30}$$

■

Corollary 4.9. *Let $G \cong \mathfrak{t}_n(w)$ be a tricyclic molecular graph with precisely seven cycles together with w pendent vertices of order $n = w+4$. Then, the following hold:*
(1) $\mathcal{LEL}(G) = \sqrt{n}+n$,
(2) $\mathcal{LEL}(\overline{G}) = 2\sqrt{n-4}+(n-4)\sqrt{n-1}$.

Proof. According to Theorem 4.8, we have that 0, 1, 4 and n are the Laplacian eigenvalues of G with multiplicities 1, $n-4$, 2 and 1, respectively. And 0, $n-4$ and $n-1$ are the Laplacian eigenvalues of $\overline{G}$ with multiplicities 2, 2 and $n-4$, respectively. Now, by using Equation (4) the result follows. ■

4.1 LE versus LEL of $\mathfrak{t}_n(r)$, $\mathfrak{t}_n(s)$, $\mathfrak{t}_n(t)$ and $\mathfrak{t}_n(w)$ and of their complements

In this section, we will give a graphical representation of the Laplacian energy (LE) and Laplacian-energy-like of the tricyclic molecular graphs, i.e., of $\mathfrak{t}_n(r)$, $\mathfrak{t}_n(s)$, $\mathfrak{t}_n(t)$ and $\mathfrak{t}_n(w)$, and of their complements, i.e., of $\overline{\mathfrak{t}_n(r)}$, $\overline{\mathfrak{t}_n(s)}$, $\overline{\mathfrak{t}_n(t)}$ and $\overline{\mathfrak{t}_n(w)}$. The main purpose of this subsection is to indicate the minimal and maximal LE and LEL of the aforementioned molecular graphs with 2000000 vertices, for this we have used python. The orange line in the graphs indicates LEL and the blue line indicates LE in the aforementioned molecular graphs. We have plotted the LE and LEL along the x-axis and the number of vertices along the y-axis.
From Figures 6, 8, 10 and 12, we observe that initially LE and LEL coincide, but when the number of vertices are increasing, then LE is increasing by LEL of $\mathfrak{t}_n(r)$, $\mathfrak{t}_n(s)$, $\mathfrak{t}_n(t)$ and $\mathfrak{t}_n(w)$. On the other hand, we face opposite situation, i.e., in Figures 7, 9, 11 and 13, we see that initially the LE and LEL coincide, but when the number of vertices are increasing, then LE is decreasing by LEL of $\overline{\mathfrak{t}_n(r)}$, $\overline{\mathfrak{t}_n(s)}$, $\overline{\mathfrak{t}_n(t)}$ and $\overline{\mathfrak{t}_n(w)}$.

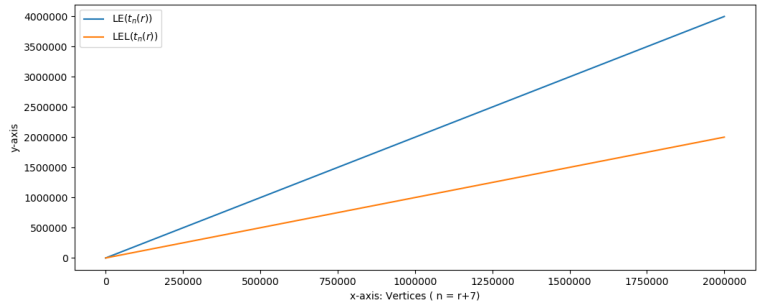

Figure 6: The LE versus LEL of the tricyclic molecular graph $\mathfrak{t}_n(r)$. The data set contains of the LE and LEL of $\mathfrak{t}_n(r)$ with n vertices, where $8 \leq n \leq 2000000$. Clearly, the data set shows that LEL is strictly less than LE for $\mathfrak{t}_n(r)$ up to 2000000 vertices.

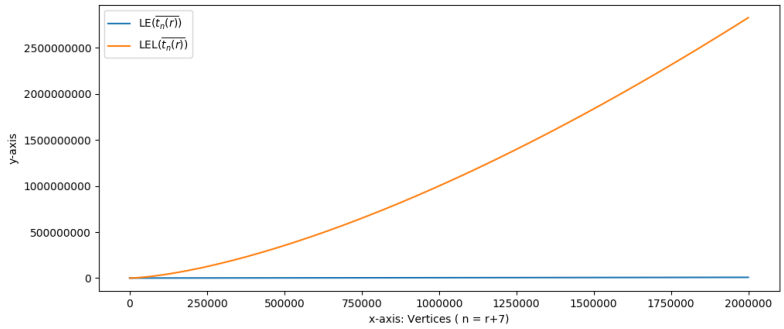

Figure 7: The LE versus LEL of the tricyclic molecular graph $\overline{\mathfrak{t}_n(r)}$. The data set consists of the LE and LEL of $\overline{\mathfrak{t}_n(r)}$ with n vertices, where $8 \leq n \leq 2000000$. Clearly, the data set shows that LE is strictly less than LEL for $\overline{\mathfrak{t}_n(r)}$ up to 2000000 vertices.

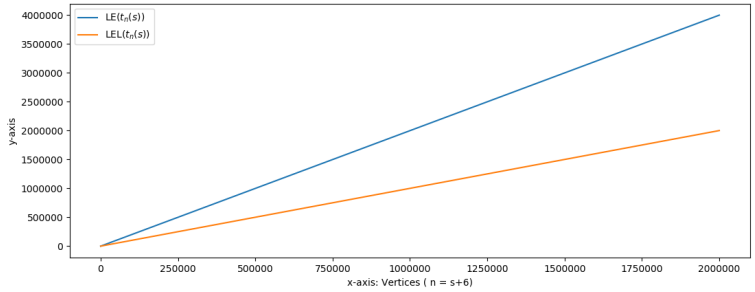

Figure 8: The LE versus LEL of the tricyclic molecular graph $\mathfrak{t}_n(s)$. The data set consists of the LE and LEL of $\mathfrak{t}_n(s)$ with n vertices, where $7 \leq n \leq 2000000$. Clearly, the data set shows that LEL is strictly less than LE for $\mathfrak{t}_n(s)$ up to 2000000 vertices.

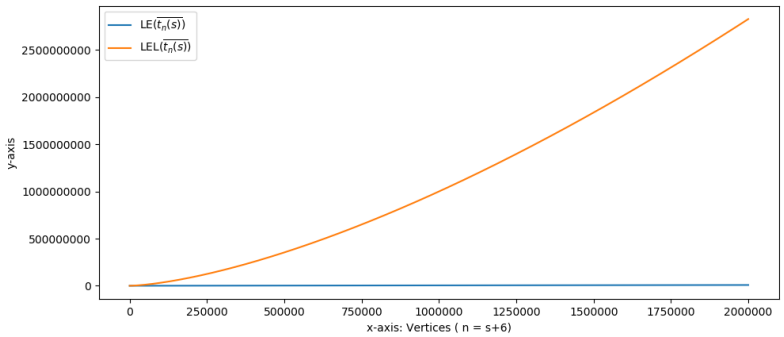

Figure 9: The LE versus LEL of the tricyclic molecular graph $\overline{\mathfrak{t}_n(s)}$. The data set consists of the LE and LEL of $\overline{\mathfrak{t}_n(s)}$ with n vertices, where $7 \leq n \leq 2000000$. Clearly, the data set shows that LE is strictly less than LEL for $\overline{\mathfrak{t}_n(s)}$ up to 2000000 vertices.

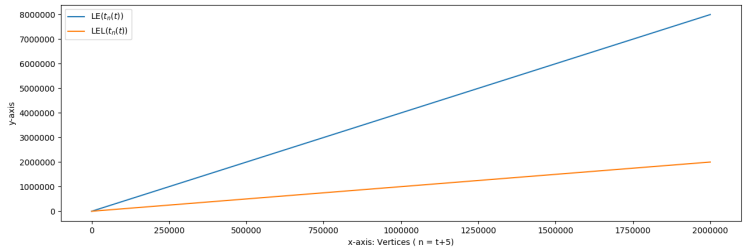

Figure 10: The LE versus LEL of the tricyclic molecular graph $\mathfrak{t}_n(t)$. The data set consists of the LE and LEL of $\mathfrak{t}_n(t)$ with n vertices, where $6 \leq n \leq 2000000$. Clearly, the data set shows that LEL is strictly less than LE for $\mathfrak{t}_n(t)$ up to 2000000 vertices.

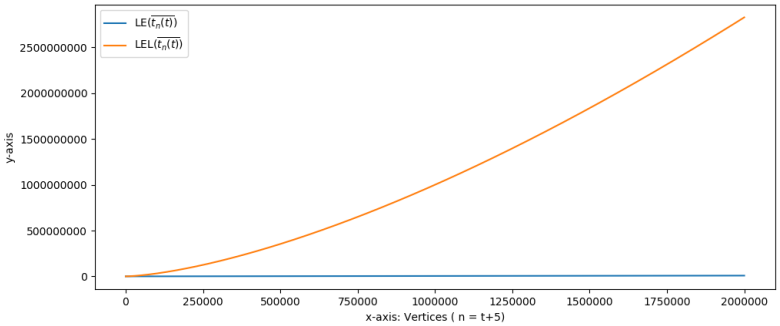

Figure 11: The LE versus LEL of the tricyclic molecular graph $\overline{\mathfrak{t}_n(t)}$. The data set consists of the LE and LEL of $\overline{\mathfrak{t}_n(t)}$ with n vertices, where $6 \leq n \leq 2000000$. Clearly, the data set shows that LE is strictly less than LEL for $\overline{\mathfrak{t}_n(t)}$ up to 2000000 vertices.

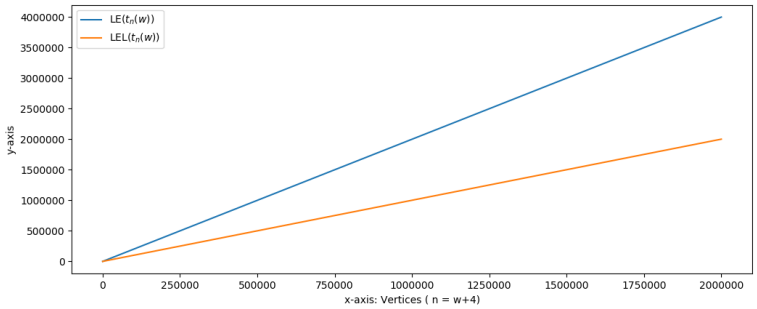

Figure 12: The LE versus LEL of the tricyclic molecular graph $\mathfrak{t}_n(w)$. The data set consists of the LE and LEL of $\mathfrak{t}_n(w)$ with n vertices, where $5 \leq n \leq 2000000$. Clearly, the data set shows that LEL is strictly less than LE for $\mathfrak{t}_n(w)$ up to 2000000 vertices.

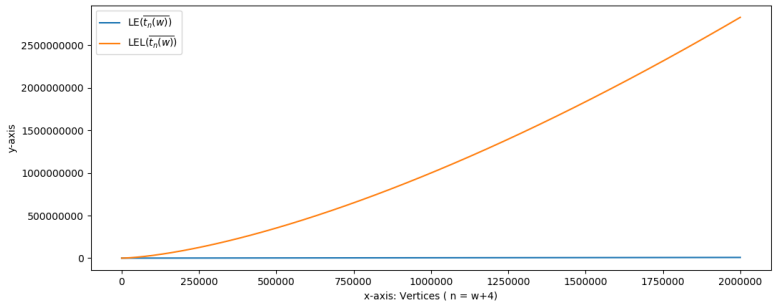

Figure 13: The LE versus LEL of the tricyclic molecular graph $\overline{\mathfrak{t}_n(w)}$. The data set consists of the LE and LEL of $\overline{\mathfrak{t}_n(w)}$ with n vertices, where $5 \leq n \leq 2000000$. Clearly, the data set shows that LE is strictly less than LEL for $\overline{\mathfrak{t}_n(w)}$ up to 2000000 vertices.

4.2 Application of LE and LEL

In addition to its classical use in chemical studies, stemming from its relation to the energy the HMO total π-electron energy, LE and LEL i.e., Equations (1), (2) and (4) have found unexpected applications in other areas of science.

The utilization of $\mathcal{LE}(G)$, $\mathcal{LEL}(G)$, and $\mathcal{E}(G)$ in QSPR/QSAR studies has been investigated in several contexts. In particular, connections between graph energies and entropy have been established. Graph-energy-related descriptors have also been employed to model biologically relevant properties of proteins. Furthermore, these measures have been applied in research on the genetic basis of Alzheimer's disease and in modeling epidemic spread. In addition, several studies have proposed biochemical applications of $\mathcal{LE}(G)$, $\mathcal{LEL}(G)$, and $\mathcal{E}(G)$. Applications of $\mathcal{LE}(G)$, $\mathcal{LEL}(G)$, and $\mathcal{E}(G)$ have also been explored in fields such as pattern recognition and image analysis, with further attempts made to employ them in medical studies of brain activity. These diverse biochemical, technical, and medical applications highlight the broader relevance of graph energies and provide justification for their development, which initially arose from abstract and theoretical mathematical considerations. Such transitions from theory to application are a recurring phenomenon in scientific research.
In Sections 3 and 4, we have obtained the exact formulas for LE and LEL for specific families of bicyclic and tricyclic molecular graphs and their complements, described in terms of the vertex count n, this means that if we have just the number of vertices for these molecular graphs then we can exactly calculate the LE and LEL immediately. In Subsections 3.1 and 4.1, we have presented the graphical interpretation of these molecular graphs and of their complements, and by these graphs we can see immediately which molecular graph has maximum and minimum LE and LEL.

5 Conclusion

In [18] Radenković and Gutman investigated the energy and LE of acyclic molecular graphs up to 14 vertices. In this paper, we have investigated the LE and LEL of some classes of bicyclic (i.e., bicyclic molecular graphs with exactly 2 and 3 cycles, respectively) and tricyclic (i.e., tricyclic molecular graphs with 3, 4, 6 and 7 cycles) molecular graphs and obtained the exact formulas for LE and LEL for these classes of graphs in terms of their orders. In Subsections 3.1 and 4.1 with the help of graphical interpretation, we showed that LE is strictly increasing while the LEL is decreasing up to 2000000 vertices. Furthermore, we showed that LE is strictly decreasing while the LEL is increasing up to 2000000 vertices for the complements of these bicyclic and tricyclic molecular graphs.

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

References

[1] I. Gutman, Total Pi-Electron energy of Benzenoid Hydrocarbons, *Topics Curr. Chem.* **162** (1992) 29–63.

[2] I. Gutman, Hyper-Wiener index and Laplacian spectrum, *J. Serb. Chem. Soc.* **68** (2003) 949–952.

[3] I. Gutman, B. Furtula, J. Đurđević, R. Kovačević and S. Stanković, Annelated perylenes: benzenoid molecules violating the Kekule-structure-based cyclic conjugation models, *J. Serb. Chem. Soc.* **70** (2005) 1023–1032.

[4] M. Perić, I. Gutman and J. Radić-Perić, The Huckel total pi-electron energy puzzle, *J. Serb. Chem. Soc.* **71** (2006) 771–783, https://doi.org/10.2298/JSC0607771P.

[5] A. Graovac, I. Gutman and N. Trinajstić, *Topological Approach to the Chemistry of Conjugated Molecules*, Springer-Verlag, Berlin, 1977.

[6] I. Gutman and O. E. Polansky, *Mathematical Concept in Organic Chemistry*, Springer-Verlag, Berlin, 1986.

[7] I. Gutman, N. Trinajstić and C. F. Wilcox, Graph theory and molecular-orbitals .XII. Acyclic Polyenes, *J. Chem. Phys.* **62** (1975) 3399–3405.

[8] W. Xiao and I. Gutman, Resistance distance and Laplacian spectrum, *Theor. Chem. Acc.* **110** (2003) 284–289, https://doi.org/10.1007/s00214-003-0460-4.

[9] B. Mohar, Laplacian matrices of graphs, *Stud. Phys. Theor. Chem.* **63** (1989) 1–8.

[10] I. Gutman and B. Zhou, Laplacian energy of a graph, *Linear Algebra Appl.* **414** (2006) 29–37, https://doi.org/10.1016/j.laa.2005.09.008.

[11] B. Zhou and I. Gutman, On Laplacian energy of graphs, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 211–220.

[12] E. Milovanović, I. Milovanović and M. Matejić, On relation between the Kirchhoff index and Laplacian-Energy-Like invariant of graphs, *Math. Interdisc. Res.* **2** (2017) 141–154, https://doi.org/10.22052/MIR.2017.85687.1063.

[13] N. De, On eccentricity version of Laplacian energy of a graph, *Math. Interdisc. Res.* **2** (2017) 131–139, https://doi.org/10.22052/MIR.2017.70534.1051.

[14] J. Liu and B. Liu, A Laplacian-energy-like invariant of a graph, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 355–372.

[15] W. Wang and Y. Luo, On Laplacian-energy-like invariant of a graph, *Linear Algebra Appl.* **437** (2012) 713–721, https://doi.org/10.1016/j.laa.2012.03.004.

[16] B. X. Zhu, The Laplacian-energy like of Graphs, *Appl. Math. Lett.* **24** (2011) 1604–1607, https://doi.org/10.1016/j.aml.2011.04.010.

[17] I. Gutman, Some properties of Laplacian eigenvectors , *Bull. Cl. Sci. Math. Nat. Sci. Math.* (2003) 1–6.

[18] S. Radenković and I. Gutman, Total π-electron energy and Laplacian energy: How far the analogy goes?, *J. Serb. Chem. Soc.* **72** (2007) 1343–1350.