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Eccentricity Laplacian energy of a graph

A. Harshitha[1,a], S. Nayak[1,b], S. D'Souza[1,c]

[1]Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal, India, 576104

[a]harshuarao@gmail.com, [b]swati.nayak@manipal.edu, [c]sabitha.dsouza@manipal.edu

Corresponding author: S. D'Souza, sabitha.dsouza@manipal.edu

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ABSTRACT Let G be a simple, finite, undirected and connected graph. The eccentricity of a vertex v is the maximum distance from v to all other vertices of G. The eccentricity Laplacian matrix of G with n vertices is a square matrix of order n, whose elements are el_{ij}, where el_{ij} is -1 if the corresponding vertices are adjacent, el_{ii} is the eccentricity of v_i for $1 \leq i \leq n$, and el_{ij} is 0 otherwise. If $\epsilon_1, \epsilon_2, \ldots, \epsilon_n$ are the eigenvalues of the eccentricity Laplacian matrix, then the eccentricity Laplacian energy of G is $ELE(G) = \sum_{i=1}^{n} |\epsilon_i - avec(G)|$, where $avec(G)$ is the average eccentricities of all the vertices of G. In this study, some properties of the eccentricity Laplacian energy are obtained and comparison between thge eccentricity Laplacian energy and the total $\pi-$electron energy is obtained.

KEYWORDS distance, eccentricity, Laplacian energy

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1. Introduction

Let G be a simple, finite, undirected and connected graph. The degree of a vertex is the number of edges incident on the vertex. The distance between two vertices is the number of edges in the shortest path between them. Eccentricity of a vertex is the maximum distance from a vertex to all other vertices of a graph. Minimum and maximum among the eccentricities of all the vertices is the radius and diameter of the graph, respectively. If the eccentricity of a vertex is equal to radius of the graph, then the vertex is called a central vertex. The set of all central vertices is called the center of the graph.

The degree of a vertex v of a graph G is denoted by $\deg_G(v)$. The notation $d_G(v_i, v_j)$ represents distance between the vertices v_i and v_j of G. Eccentricity of a vertex v is denoted by $e_G(v)$. The notations $r(G)$ and $d(G)$ represent the radius and the diameter of the graph respectively. The center of the graph is denoted by $C(G)$.
The average eccentricity of a graph is as follows

$$avec(G) = \frac{1}{n} \sum_{i=1}^{n} e_G(v_i).$$

The status of a vertex v_i is given by

$$\sigma_G(v_i) = \sum_{v_j \in V(G)} d_G(v_i, v_j).$$

A clique of a graph is an induced subgraph which is complete. The size of the largest clique is the clique number of the graph, denoted by ω. The independent set of a graph is the subset of the set of vertices in which no two vertices are adjacent. The independent number of a graph is the cardinality of the maximum independent set of vertices, denoted by α.

The energy of a graph was introduced by I. Gutman [1] in 1978 as sum of the absolute eigenvalues of the adjacency matrix associated with the graph. That is, if $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of the adjacency matrix of the graph G, then the energy of G is as follows

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

The spectrum of the graph G with distinct eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_k$ having multiplicity $m_1, m_2, \ldots, m_k$, respectively, is denoted by

$$Spec(G) = \begin{pmatrix} \lambda_1 & \lambda_2 & \lambda_3 & \ldots & \lambda_k \\ m_1 & m_2 & m_3 & \ldots & m_k \end{pmatrix}.$$

In 2006, I Gutman and B. Zhou [2] introduced the Laplacian energy of a graph. The Laplacian matrix of a graph on n vertices is the square matrix of order n, whose diagonal entries are degrees of the corresponding vertices and non-diagonal entries are -1 if the corresponding vertices are adjacent and 0 if the corresponding vertices are non-adjacent. If $\mu_1, \mu_2, \ldots, \mu_n$ are the eigenvalues of the Laplacian matrix, then the Laplacian energy of G of order n and size m is given by the expression

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

Motivated by the works on Laplacian energy [3–7], in this paper, the eccentricity Laplacian matrix is considered and its spectral properties are studied.

The eccentricity Laplacian matrix of a connected graph G on n vertices, denoted by $EL(G)$ [8], is a square matrix of order n, whose elements are given by el_{ij}, where

$$el_{ij} = \begin{cases} -1 & \text{if } v_i \sim v_j \text{ and } i \neq j \\ e_G(v_i) & \text{if } i = j \\ 0 & \text{otherwise.} \end{cases}$$

The trace of the matrix $EL(G)$ is $Tr(EL(G)) = \sum_{i=1}^{n} e_G(v_i) = n(avec(G))$. If $\epsilon_1, \epsilon_2, \ldots, \epsilon_n$ are the eigenvalues of the matrix $EL(G)$, then the eccentricity Laplacian energy is defined as

$$ELE(G) = \sum_{i=1}^{n} \left| \epsilon_i - avec(G) \right|.$$

It is well known that the energy of a graph coincides with the total $\pi-$electron energy of conjugated hydrocarbon molecule. Also, few comparisons between different energies and total $\pi-$electron energy can be found in [9–11]. In a similar manner, in this study, comparison between the eccentricity Laplacian energy and the total $\pi-$electron energy of hydrocarbons are made. The result of which gives the strong correlation between the two energies.

2. Preliminaries

Theorem 1. *[12] For any connected graph G,*

$$avec(G) \leq \frac{1}{n}\sigma_G(C(G)) + r(G).$$

The equality holds for any tree.

Theorem 2. *[12] For a connected graph of order n,*

$$avec(G) \leq \frac{1}{n} \left\lfloor \frac{3}{4}n^2 - \frac{1}{2}n \right\rfloor.$$

The equality holds if and only if $G \cong P_n$.

Theorem 3. *[13] Let $G(\ncong K_n)$ be a connected graph of order n with clique number ω and independent number α. Then*

$$avec(G) \geq \frac{1}{n}(\omega + 2\alpha - 1).$$

Theorem 4. *[13] Let $G(\ncong K_n)$ be a connected graph of order n with clique number ω. Then $\sum_{i=1}^{n} e_G^2(v_i) \geq 4n - 3\omega + 3$.*

3. Main Results

Lemma 1. *The matrix $EL(G)$ is positive semi-definite if $e_G(v_i) \geq deg_G(v_i)$ for all $i = 1, 2, \ldots, n$.*

Proof. In a graph G of order n, if $e_G(v_i) \geq deg_G(v_i)$ for all $i = 1, 2, \ldots, n$, then $EL(G)$ is symmetrically diagonally dominant matrix and therefore a positive semi-definite matrix. □

Lemma 2. *Let G be a connected graph on n vertices. Then $ELE(G) = E(G)$ if $e_G(v_i) = k$ for all $v_i \in V(G)$ and $k \in \mathbb{Z}$.*

Proof. If $e_G(v_i) = k$ for all $v_i \in V(G)$, then $EL(G) = -A(G) + kI_n$ and $e_i(G) = -\lambda_i(G) + k$ and $avec(G) = k$

$$\begin{aligned} ELE(G) &= \sum_{i=1}^{n} |-\lambda_i(G) + k - k| \\ &= \sum_{i=1}^{n} |\lambda_i(G)| = E(G). \end{aligned}$$

□

Table 3 gives one some graphs with equal adjacency energy and eccentricity Laplacian energy.

TABLE 1. Graphs with equal adjacency energy and eccentricity Laplacian energy

Graph	**Eccentricities of all the vertices**
complete graph K_n	1
cycle C_n	$\lfloor \frac{n}{2} \rfloor$
complete bipartite graph $K_{m,n}$, $m \leq n$, $m > 1$	2
cocktail party graph $K_{n\times 2}$	2
crown graph S_n^0	3

Remark. $ELE(G) = LE(G) = E(G)$ if $e_G(v_i) = \deg_G(v_i)$ for all $v_i \in V(G)$.

For instance, among the graphs in table 3 complete graph K_2, cycle C_4, complete bipartite graph $K_{2,2}$, cocktail party graph $K_{2\times 2}$, and crown graph S_4^0 have equal energy, Laplacian energy, and eccentricity Laplacian energy.

Theorem 5. *Let G be a connected graph of order n, size m with clique number ω and independent number α. Then*

$$ELE \geq \sqrt{2mn + Mn + N^2 - 2\left\{\left\lfloor \frac{3}{4}n^2 - \frac{1}{2}n \right\rfloor\right\}^2}.$$

Here $M = 4n - 3\omega + 3$ and $N = \omega + 2\alpha - 1$.

Proof. Let $\epsilon_1 \geq \epsilon_2 \geq \ldots \geq \epsilon_n$ be the eigenvalues of $EL(G)$. Consider the Cauchy-Schwartz inequality,

$$(\sum_{i=1}^{n} a_i b_i)^2 \leq (\sum_{i=1}^{n} a_i^2)(\sum_{i=1}^{n} b_i^2).$$

Set $a_i = 1$ and $b_i = |\epsilon_i - avec(G)|$, then

$$(ELE(G))^2 = \left(\sum_{i=1}^{n} |\epsilon_i - avec(G)|\right)^2 \leq n \sum_{i=1}^{n} |\epsilon_i - avec(G)|^2 .$$

However,

$$\sum_{i=1}^{n} |\epsilon_i - evec(G)|^2 = \sum_{i=1}^{n} \epsilon_i^2 + \sum_{i=1}^{n} (avec(G))^2 - 2avec(G) \sum_{i=1}^{n} \epsilon_i. \tag{1}$$

Now we will find the values of $\sum_{i=1}^{n} \epsilon_i^2$, $\sum_{i=1}^{n} (avec(G))^2$ and $avec(G) \sum_{i=1}^{n} \epsilon_i$. Consider

$$\begin{aligned} \sum_{i=1}^{n} \epsilon_i^2 &= \sum_{i=1}^{n} (EL(G))_{ii}^2 \\ &= 2m + \sum_{i=1}^{n} e_G^2(v_i). \end{aligned}$$

But, $\sum_{i=1}^{n} e_G^2(v_i) \geq 4n - 3\omega + 3$ (by Theorem 4). Therefore,

$$\sum_{i=1}^{n} \epsilon_i^2 \geq 2m + 4n - 3\omega + 3. \tag{2}$$

By Theorem 3, $avec(G) \geq \frac{\omega+2\alpha-1}{n}$ and therefore,

$$\sum_{i=1}^{n}(avec(G))^2 \geq \frac{(\omega+2\alpha-1)^2}{n}. \tag{3}$$

and by Theorem 2 and noting the fact that $\sum_{i=1}^{n}\epsilon_i = n(avec(G))$, one obtains

$$-2avec(G)\sum_{i=1}^{n}\epsilon_i \geq \frac{-2}{n}\left\{\left\lfloor \frac{3}{4}n^2 - \frac{1}{2}n \right\rfloor\right\}^2. \tag{4}$$

Theorem 5 follows by substituting the values of equations 2, 3, and 4 in equation 1. □

Theorem 6. *Let G be a connected graph of order n, size m with clique number ω, independent number α, and radius $r(G)$. Then*

$$ELE(G) \leq \Big\{2mn + n^2(r(G)^2) + r(G) + 2r(G)\sigma_G(C(G)) + n\sum_{i=1}^{n}(d_G(u, C(G)))^2 + (\sigma_G(C(G)))^2 - 2R^2\Big\}^{\frac{1}{2}}.$$

Here $R = \omega + 2\alpha - 1$ and $\sigma_G(C(G))$ is the status of the center of G.

Proof. Let v be a vertex of a connected graph G. Note that $e_G(v) \leq nr(G) + \sigma_G(C(G))$ and the equality holds for any tree [12]. Let $\epsilon_1 \geq \epsilon_2 \geq \ldots \geq \epsilon_n$ be the eigenvalues of $EL(G)$. Then by the Cauchy-Schwartz inequality,

$$\begin{aligned}(ELE(G))^2 &= \left(\sum_{i=1}^{n}|\epsilon_i - avec(G)|\right)^2 \\ &\leq n\sum_{i=1}^{n}|\epsilon_i - avec(G)|^2 \\ &= \sum_{i=1}^{n}\epsilon_i^2 + \sum_{i=1}^{n}(avec(G))^2 - 2avec(G)\sum_{i=1}^{n}\epsilon_i. \end{aligned} \tag{5}$$

Now we will find the values of $\sum_{i=1}^{n}\epsilon_i^2$, $\sum_{i=1}^{n}(avec(G))^2$ and $avec(G)\sum_{i=1}^{n}\epsilon_i$. Consider

$$\sum_{i=1}^{n}\epsilon_i^2 = 2m + \sum_{i=1}^{n}e_G^2(v_i).$$

Noting the fact that $e_G(v_i) \leq r(G) + d_G(v_i, C(G))$, one comes to the inequality

$$\sum_{i=1}^{n}\epsilon_i^2 \leq 2m + n(r(G))^2 + 2r(G)\sigma_G(C(G)) + \sum_{i=1}^{n}(d_G(u, C(G)))^2. \tag{6}$$

Also

$$\sum_{i=1}^{n}(avec(G))^2 \leq \frac{(nr(G) + \sigma_G(C(G)))^2}{n}. \tag{7}$$

By lemma 3, $avec(G) \geq \omega + 2\alpha - 1$ which implies that

$$-2avec(G)\sum_{i=1}^{n}\epsilon_i \leq \frac{-2}{n}(\omega+2\alpha-1)^2. \tag{8}$$

Theorem 6 follows by substituting the values of 6, 7 and 8 in 5. □

4. Eccentricity Laplacian matrix of a tree

Theorem 7. *Let T be a tree on n vertices. Let $f_n(T,\lambda) = a_0\lambda^n + a_1\lambda^{n-1} + a_2\lambda^{n-2} + \cdots + a_n$ be the characteristic polynomial of $EL(T)$. Then,*

(1) $a_0 = 1$.
(2) $a_1 = -(nr(T) + \sigma_T(C(T)))$.
(3) $a_2 = \frac{(r(T))^2 n(n-1)}{2} - (n-1) + \sum_{i=1}^{n-1} x_i(x_{i+1} + x_{i+2} + \cdots + x_n) + \sum_{i=1}^{n}(n-1)x_i$, *where,* $x_i = r(T) + d(v_i, C(T))$.

Proof. (1) By the definition of $f_n(T,\lambda)$, $a_0 = 1$.

(2) The value of a_1 is (-1) times the sum of the determinants of all 1×1 principal sub-matrices of $EL(T)$. By lemma 1, $avec(T) = \frac{1}{n}\sigma_T(C(T)) + r(T)$. Therefore, $a_1 = -(nr(T) + \sigma_T(C(T)))$.

(3) The value of a_2 is sum of the determinants of all 2×2 principal sub-matrices of $EL(T)$. That is,

$$a_2 = \sum_{1\le i<j\le n} \begin{vmatrix} el_{ii} & el_{ij} \\ el_{ji} & el_{jj} \end{vmatrix} = \sum_{1\le i<j\le n} el_{ii}el_{jj} - \sum_{1\le i<j\le n} el_{ij}^2.$$

But, $\sum_{1\le i<j\le n} el_{ii}el_{jj} = \frac{(r(T))^2 n(n-1)}{2} + \sum_{i=1}^{n-1} x_i(x_{i+1}+x_{i+2}+\cdots+x_n) + \sum_{i=1}^{n}(n-1)x_i$ and $\sum_{1\le i<j\le n} el_{ij}^2 = n-1$ and Theorem 7 follows by substitution.

□

Theorem 8. *Let T be a tree on n vertices with radius $r(T)$ and center $C(T)$. Then*

$$\begin{aligned} ELE(T) \le \big\{ & n(nr^2(T) + (d_T(u_i, C(T)))^2 + 2r(T)\sigma_T(C(T)) + 2n - 2) \\ & -(nr(T) + \sigma_T(C(T)))^2 \big\}^{\frac{1}{2}}. \end{aligned}$$

Proof. Let $\epsilon_1 \ge \epsilon_2 \ge \ldots \ge \epsilon_n$ be the eigenvalues of $EL(T)$. Consider the Cauchy-Schwartz inequality

$$(\sum_{i=1}^{n} a_i b_i)^2 \le (\sum_{i=1}^{n} a_i^2)(\sum_{i=1}^{n} b_i^2).$$

Set $a_i = 1$ and $b_i = |\epsilon_i - avec(T)|$, then

$$\begin{aligned} (ELE(T))^2 &= \left(\sum_{i=1}^{n} |\epsilon_i - avec(T)|\right)^2 \\ &\le n\sum_{i=1}^{n} |\epsilon_i - avec(T)|^2 \\ &= n\left(\sum_{i=1}^{n} \epsilon_i^2\right) + \sum_{i=1}^{n}(avec(T))^2 - 2avec(T)\sum_{i=1}^{n}\epsilon_i. \end{aligned}$$

But $e_T(u_i) = r(T) + d_T(u_i, C(T))$ and therefore, $avec(T) = nr(T) + \sigma_T(C(T))$ and $\epsilon_i^2 = nr^2(T) + 2r(T)\sigma_T(C(T)) + \sum_{i=1}^{n} d_T^2(u_i, C(T)) + 2n - 2$. Therefore,

$$\begin{aligned} (ELE(T))^2 \le\, & n(nr^2(T) + 2r(T)\sigma_T(C(T)) + (d_T(u_i, C(T)))^2 + 2m) \\ & - (nr(T) + \sigma_T(C(T))^2) \end{aligned}$$

and the proof follows. □

Theorem 9. *Let S_n be a star graph on n vertices. Then,*

$$ELE(S_n) = \frac{n-2}{n} + \sqrt{4n-3}.$$

Proof. The average eccentricity of star graph S_n is $2n - 1$. Consider

$$|\gamma I - EL(S_n)| = \left| \begin{pmatrix} \gamma-1 & 1 & 1 & 1 & \cdots & 1 & 1 \\ 1 & \gamma-2 & 0 & 0 & \cdots & 0 & 0 \\ 1 & 0 & \gamma-2 & 0 & \cdots & 0 & 0 \\ 1 & 0 & 0 & \gamma-2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 0 & 0 & 0 & \cdots & \gamma-2 & 0 \\ 1 & 0 & 0 & 0 & \cdots & 0 & \gamma-2 \end{pmatrix} \right|.$$

The characteristic polynomial of $EL(S_n)$ is $(\gamma-2)^{n-2}(\gamma^2-3\gamma-(n-3))$ and the eccentric Laplacian spectrum of S_n is

$$\begin{pmatrix} 2 & \frac{3+\sqrt{4n-3}}{2} & \frac{3-\sqrt{4n-3}}{2} \\ n-2 & 1 & 1 \end{pmatrix}.$$

Therefore,

$$ELE(S_n) = \frac{n-2}{n} + \sqrt{4n-3}.$$

□

5. Chemical significance of the eccentric Laplacian energy

The eccentric Laplacian energies of Polyenes, Vinyl compounds, Polyacenes and Cyclobutadienes listed in the Dictionary of $\pi-$electron calculation [14] are calculated and compared with the respective total $\pi-$electron energies when $S=0$, where S is a overlap integral. Refer [14] for more details regarding terminologies related to total $\pi-$electron energy (Figs. 1, 2).

When the eccentric Laplacian energy of Polyenes and Vinyl compounds are compared with the total $\pi-$electron energy, very strong correlation has been found with correlation coefficient 0.96 (Figs. 3, 4).

Similarly, the eccentric Laplacian energies of Polyacenes and Cyclobutadienes are compared with the total $\pi-$electron energy, which gives correlation coefficient 0.98 (Figs. 5, 6).

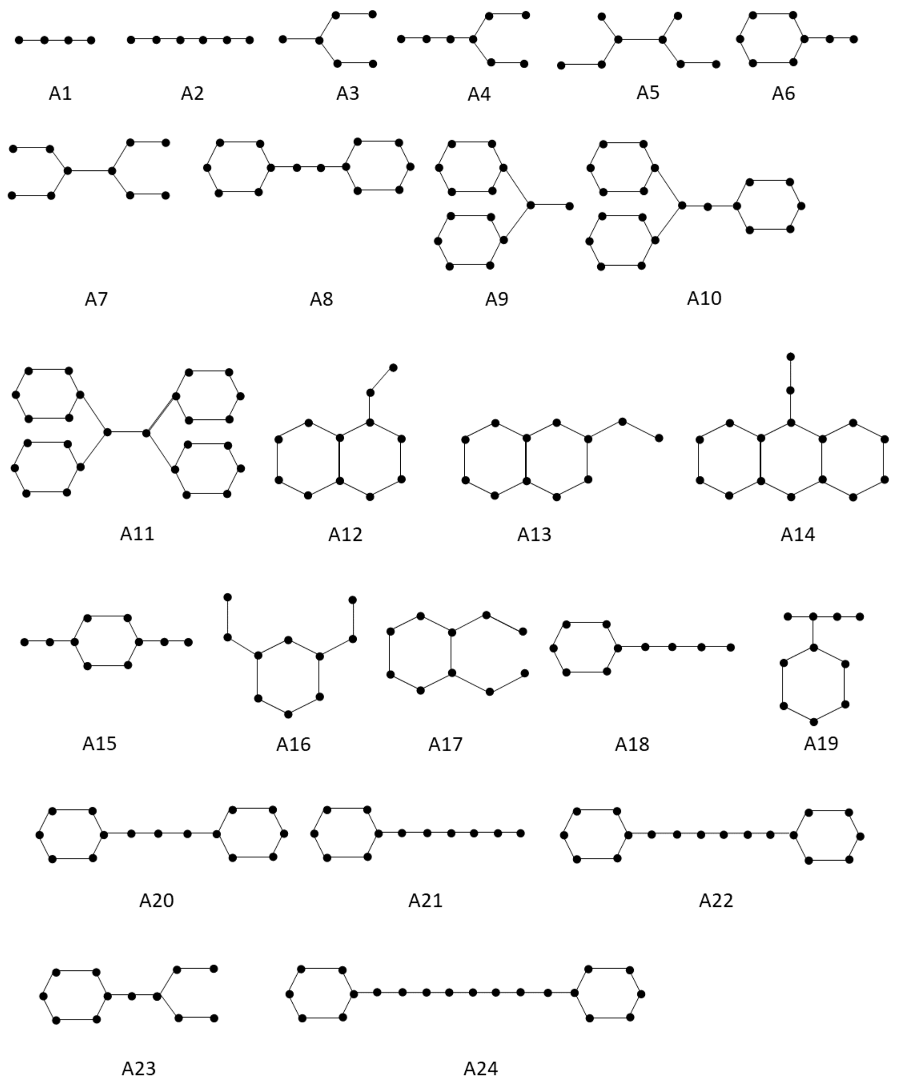

FIG. 1. Polyenes and vinyl compounds

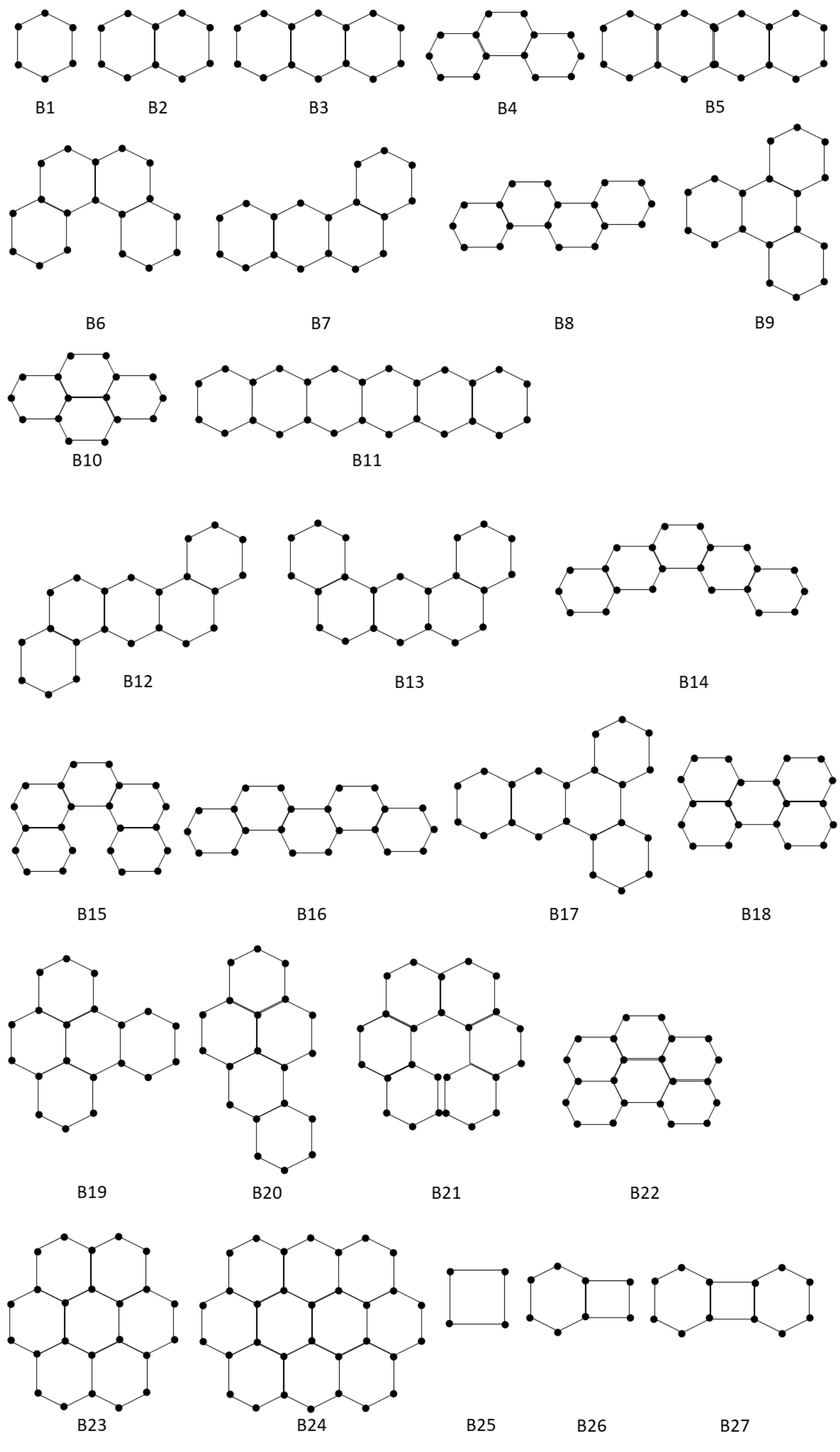

FIG. 2. Polyacenes and Cyclobutadienes

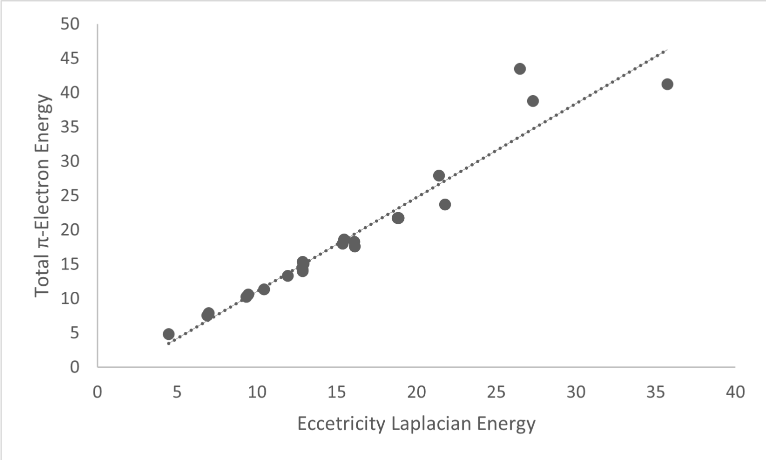

FIG. 3. Scatter plot of $ELE(G)$ and total $\pi-$electron energy of Polyenes and Vinyl compounds

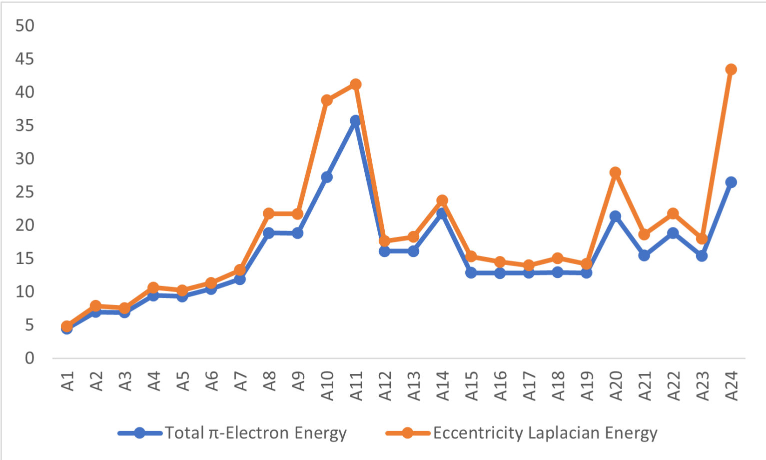

FIG. 4. Comparison between $ELE(G)$ and total $\pi-$electron energy of Polyenes and Vinyl compounds

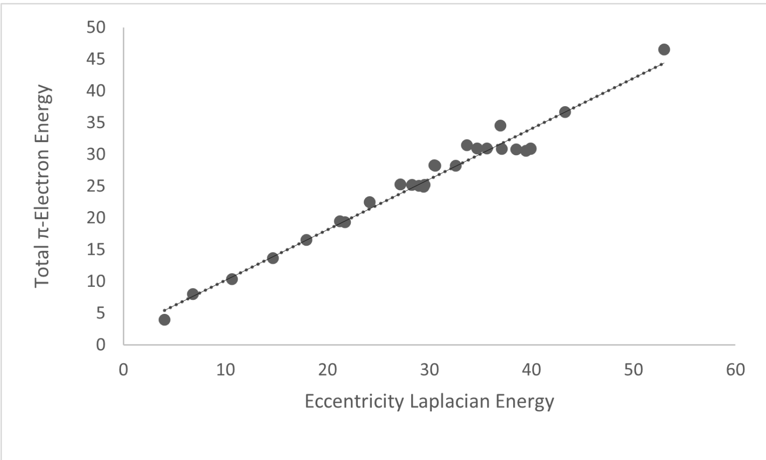

FIG. 5. Scatter plot of $ELE(G)$ and total $\pi-$electron energy of Polyacenes and Cyclobutadienes

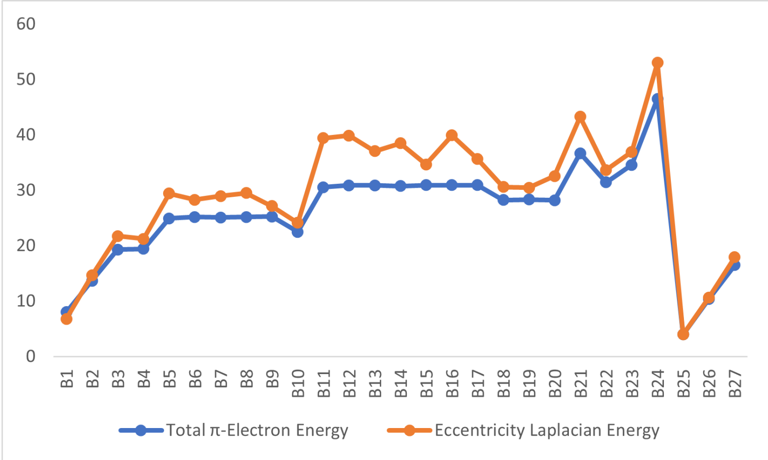

FIG. 6. Comparison between $ELE(G)$ and total $\pi-$electron energy of Polyacenes and Cyclobutadienes

6. Conclusion

In this study, the eccentricity Laplacian matrix $EL(G)$ of a graph G is explored and the corresponding eccentricity Laplacian energy $ELE(G)$ is derived. This analysis includes conditions under which $EL(G)$ is positive semi-definite and scenarios where $ELE(G)$ matches the ordinary and the Laplacian energies of the graph. We also established several bounds for $ELE(G)$ in relation with various graph parameters, such as the number of vertices and edges, the clique number, the independent number, the radius, and the status of the center.

Additionally, we characterized the eccentricity Laplacian matrix and its energy specifically for trees. As an intriguing application, we compared the eccentricity Laplacian energy of specific polyenes, vinyl compounds, polyacenes, and cyclobutadienes with their total π-electron energies. Remarkably, the correlation coefficient between $ELE(G)$ and the total π-electron energies is found to be 0.96 for polyenes and vinyl compounds, and 0.98 for polyacenes and cyclobutadienes, demonstrating a very strong correlation.

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Information about the authors:

A. Harshitha – Department of Mathematics, Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal, India, 576104; harshuarao@gmail.com

S. Nayak – Department of Mathematics, Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal, India, 576104; swati.nayak@manipal.edu

S. D'Souza – Department of Mathematics, Manipal Institute of Technology, Manipal Academy of Higher Education, Manipal, India, 576104; sabitha.dsouza@manipal.edu

Conflict of interest: the authors declare no conflict of interest.