BALANCED LAPLACIAN ENERGY OF ORGANIC COMPOUND ALKANES

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Abstract:

Let G be a simple and signed graph with order n and size m. The signed Laplacian is defined by $\bar{L} = \overline{D} - W$, where $\bar{D}$ is the signed degree matrix and W is a symmetric matrix with zero diagonal entries. The signed Laplacian is a symmetric positive semidefinite. Let $\mu_1 \geq \mu_2 \geq \mu_3 \geq \ldots. \mu_n$ be the eigen values of the Laplacian matrix. The signed Laplacian energy is defined as $\sum_{i=1}^{n} \left|\mu_i - \frac{2m}{n}\right|$. In this paper, we adopted the adjacency and degree matrices that described the structure of an alkane for which a method is outlined using simple matrix algebra. Additionally, the calculations offer a picture of the relative branched value for each carbon atom and hydrogen atom of the alkane. Also we found the balanced laplacian energy of alkanes and attained their bounds.

Keywords:

Signed Laplacian Matrix, Balanced Laplacian energy, Organic compound alkanes.

1.Introduction:

Alkanes are chemical compounds that consist of carbon (C) and hydrogen (H) atoms, so they are also called hydrocarbons. The chemical structure of alkanes only consists of single bonds. Almost all other organic compounds can be named as derivatives of these simple hydrocarbons which have long carbon chains and are often called paraffins in chemical industry. The most simple alkane is methane with the formula CH_4. The second alkane is ethane with the formula C_2H_6 and the formula of n-th alkanes is C_nH_{2n+2}. [4, 5, 17, 18, 20]

An adjacency matrix is a matrix which describes the adjacent vertices in a graph G. If G is a graph of order n, then its adjacency matrix is a (nxn) square matrix and is defined as

$$a_{ij} = \begin{cases} 1 \; if \; v_i is \; adjacent \; to \; v_j \\ 0 \; otherwise \end{cases}$$

The eigenvalues $\boldsymbol{\lambda}_1, \boldsymbol{\lambda}_2, \ldots\ldots, \boldsymbol{\lambda}_n$ of A is assumed in non increasing order and they are the eigenvalues of the graph G. The energy E(G) of G is defined as sum of the absolute values of the eigenvalues of G. i.e., E(G) = $\sum |\lambda i|$. A Signed graph is a graph with the additional structure that edges are given a sign of either +1 or -1. Formally, a signed graph is a pair

$\sum = (\Gamma, \sigma)$ consisting of an underlying graph $\Gamma = (V,E)$ and a signature $\sigma : E \rightarrow \{+1,-1\}$.

The Laplacian matrix of the graph G denoted by L(G) = D(G) - A(G) is a square matrix of order n, where D(G) is the diagonal matrix of vertex degrees of the graph G and A(G) is the adjacency matrix. Let $\mu_1 \geq \mu_2 \geq \mu_3 \geq \ldots. \mu_n$ form the Laplacian spectrum of the Laplacian matrix G then the Laplacian energy LE(G) of G is

defined as $\sum_{i=1}^{n}\left|\mu_i - \frac{2m}{n}\right|$[6,7,8,10]. Let G = (V, W) be a signed graph whose underlying graph is connected. Then G is balanced if there is a partition of its vertex set V into two clusters V_1 and V_2 such that all the positive edges connect vertices within V_1 or V_2 and all the negative edges connect vertices between V_1 and V_2. If the signed graph has an even number of negative edges then it is called a Balanced Signed graph. Here, we applied the concept of balanced graph into the organic compound alkanes and we found the balanced Laplacian energy and their bounds.[1, 2, 3, 11, 12]

2. Definitions :

2.1 Alkanes :

Alkanes are the simplest organic compounds consisting of only hydrogen and carbon atoms with only single bonds between carbon atoms the general chemical formula of alkane is calculated by $C_n\ H_{2n+2}$. Alkane are also called as saturated hydrocarbon which includes monocyclic or polycyclic molecules.

2.2 Marked graph:

A marked graph is a signed graph where every vertex has a "sign" + or -.

2.3 Signed graph:

A Signed graph is just an ordinary graph with each of its edges labelled with either + or a – . In the area of graph theory in Mathematics, a signed graph is a graph in which each edge has a positive or negative sign.

2.4 Balanced signed graph:

If G = (V,E) be a signed graph,then G is balanced if it is possible to partition V into two subsets A,B such that, positive edges have both ends in A or both ends in B. The negative edges have one end in A and the other end in B. The graph contains an even number of -ve sign. So this graph is a balanced signed graph.

2.5 Laplacian Matrix :

Given a simple graph G with order n, its Laplacian matrix $L_{(n\times n)}$ is defined as L = D – A, Where D is the degree matrix and A is the adjacency matrix of the graph. The adjacency marix A contains only 1's or 0's and its diagonal elements are all 0's. In the case of directed graphs either the indegree or outdegree could be used. Now, L = (L_{ij}) is defined as follows:

$$L_{ij} = \begin{cases} -1\ if\ v_i\ is\ adjacent\ to\ v_j \\ 0\ if\ v_i\ is\ adjacent\ to\ v_j \\ d_i\ if\ v_i = v_j \end{cases}$$

Where d_i is the degree of vertex v_i.

3. Structural formulae :

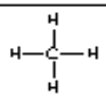
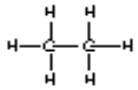
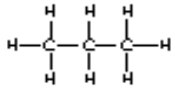
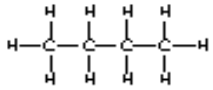
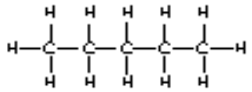
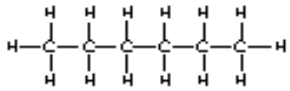
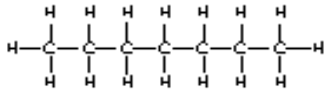
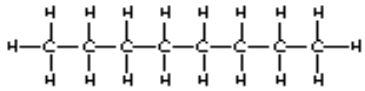
Hydrocarbons with only carbon-to-carbon single bonds (C–C) and existing as a continuous chain of carbon atoms also bonded to hydrogen atoms are called alkanes. In alkane molecules, the additional carbon atoms are attached to each other by single covalent bonds. Each carbon atom is also attached to sufficient hydrogen atoms to produce a total of four single covalent bonds about itself. Methane (CH_4), ethane (C_2H_6), and propane (C_3H_8) are the

beginning of a series of compounds in which any two members in a sequence differ by one carbon atom and two hydrogen atoms—namely, a CH_2 unit. The first 10 members of this series are given below.

List of Alkane :

- Methane (CH_4)
- Ethane (C_2H_6)
- Propane (C_3H_8)
- Butane (C_4H_{10})
- Pentane (C_5H_{12})
- Hexane (C_6H_{14})
- Heptane (C_7H_{16})
- Octane (C_8H_{18})
- Nonane (C_9H_{20})
- Decane ($C_{10}H_{22}$)

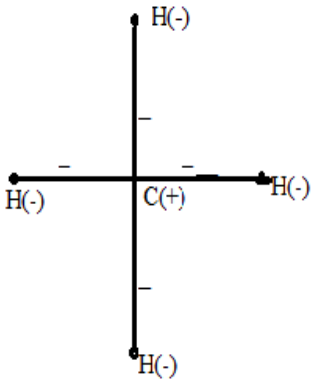
3.1 : Structures of Alkanes:

# Carbons	Name	Structure
1	methane	
2	ethane	
3	propane	
4	butane	
5	pentane	
6	hexane	
7	heptane	
8	octane	

4. Comparison between chemical compound alkanes with Balanced signed graph:

Alkanes contains naturally carbon and hydrogen atoms where carbon atom has +ve sign and hydrogen atom has - ve sign. A marked graph is a simple graph where every vertex has a sign + or - . We applied these concepts in the structure of alkanes. The structure of alkanes is compared with graphical structure of a tree. So,the vertex of hydrogen atoms are pendent and carbon atom has degree four. Therefore, the vertex of carbon atom has +ve sign and hydrogen atom has - ve sign . By taking the sign of each edge to be the product of the signs of its adjacent vertices, the vertex set of this graph is partitioned into two clusters. One cluster contain carbon atoms and another cluster contains hydrogen atoms. Any edge between the two vertices has the product of their signs. So this type of graph contains even number of negative edges . So these graphs are called balanced signed graphs. For example, the chemical compound Methane CH_4 has totally five vertices , one is +ve and the four are – ve. The following figure is the balanced signed graph of the chemical compound Methane. [9,12]

Structure of Methane:



The Balanced Laplacian matrix of the alkane Methane is as follows:

$$\bar{L}\,\mathbf{E}\,(\mathbf{M}) = \begin{pmatrix} 4 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

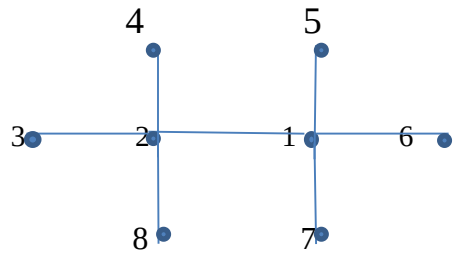
The Characteristic equation is $\mu^5 - 8\mu^4 + 18\mu^3 - 16\mu^2 + 5\mu = 0$

The Eigenvalues are 0.0000, 1.0000,1.0000, 1.0000, 5.0000 and the

Average degree is 1.6

The Balanced Laplacian Energy of the Methane is 7 approximately.

Structure of Ethane:



The Balanced Laplacian matrix of the alkane Ethane is as follows:

$$\bar{L}E(E) = \begin{pmatrix} 4 & -1 & 0 & 0 & 1 & 1 & 1 & 0 \\ -1 & 4 & 1 & 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

The Characteristic equation is $\mu^8 - 14\mu^7 + 72\mu^6 - 176\mu^5 + 229\mu^4 - 162\mu^3 + 58\mu^2 - 8\mu = 0$

The Eigenvalues are 0.0000, 0.3542 ,1.0000, 1.0000, 1.0000,1.0000, 4.0000 , 5.6458 and the Average degreeis 1.75

The Balanced Laplacian Energy of the Ethane is 12 approximately.

It follows that t he Balanced Laplacian matrix of propane is

$$\bar{L}E(P) = \begin{pmatrix} 4 & -1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 \\ -1 & 4 & -1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & -1 & 4 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

The Characteristic equation is

μ^{11}- 20 μ^{10} + 162 μ^{9} - 696 μ^{8} + 1761 μ^{7} - 2772 μ^{6} + 2775 μ^{5} – 1752 μ^{4} + 666 μ^{3} - 136μ^{2}

+11 μ =0.

The Eigenvalues are0.0000, 0.2087,0.5226 , 1.0000,1.0000, 1.0000,1.0000 ,1.0000, 3.5519, 4.7913, 5.9254

Average degree is 1.8

So the Balanced Laplacian Energy of the Propane is 16 approximately

Proceeding like this, it is generalised that the Balanced Laplacian energy of any alkane is $\frac{3n-1}{2}$ approximately.

5. Observations:

5.1 Cayley's Theorem: [17, 20]

$C_n H_{2n+2}$ alkanes structure is a tree

5.2 Let G be a graph with n ≥ 4 vertices. then

$LE(G) \leq \mu_1 - \mu_{n-1} + d(G) + \sum_{i=2}^{n-2} max\{\mu i, d(G)\}$ [14]

5.3 If G be a tree, then (i) $\frac{\mu_n}{\mu_2} + \frac{\mu_2}{\mu_n} \geq \frac{(n-1)}{m}(2 + \frac{4m}{n})$. [13]

(ii) $\frac{\mu_n}{\mu_2} + \frac{\mu_n}{\mu_2} \geq 4 - \frac{4}{n}$.

5.4 (i) Let G be a tree with n vertices, of which p are pendent vertices, where $2 \leq p \leq n-1$. Then $LE(G) < E(G) + 2p\left(1 - \frac{2}{n}\right)$.

(ii) Let G be a unicyclic graph with n vertices, of which p are pendent vertices, where $0 \leq p \leq n-3$. Then $LE(G) \leq E(G) + 2p$ with equality if and only if p = 0. [15]

5.6 The Matrix Tree Theorem: [20]

Given a graph G, its adjacency matrix A, and its degree matrix D, then the number of non identical spanning trees of G is equal to the value of any cofactor of the matrix D – A.

6.BOUNDS OF BALANCED LAPLACIAN ENERGY OF ALKANE:

From the above results, we found the lower bound and upper bound for Balanced Laplacian Energy of Alkanes

Theorem:6.1 Consider an Alkane with order n (= 5,8,11 … 32) out of which there are p = $\frac{2(n+1)}{3}$ pendent vertices where $4 \leq p \leq n-1$ then $\bar{L}E(G) \leq E(G) + \frac{4(n+1)(n-2)}{3n}$.

Proof:

Any Alkane G is a chemical molecule then by theorem 5.1, G is a tree with n (= 5,8,11…) vertices and the number of pendent vertices is $\frac{2(n+1)}{3}$

From 5.4, $\bar{L}E(G) \leq E(G) + 2p\left(1 - \frac{2}{n}\right)$.

$\bar{L}E(G) \leq E(G) + 2.\frac{2(n+1)}{3}\left(1 - \frac{2}{n}\right)$.

$$\bar{L}E(G) \leq E(G) + \frac{4(n+1)}{3}\left(\frac{n-2}{n}\right).$$

$$\bar{L}E(G) \leq E(G) + \frac{4(n+1)(n-2)}{3n}.$$

Theorem: 6.2

Consider an Alkane with order n (= 5,8,11 … 32) and size n-1, then $\frac{\mu_n}{\mu_2} + \frac{\mu_2}{\mu_n} \geq \frac{2(3n-2)}{n}$.

Proof:

From 5.2, $\frac{\mu_n}{\mu_2} + \frac{\mu_2}{\mu_n} \geq \frac{(n-1)}{m}(2 + \frac{4m}{n})$.

$$\geq \frac{(n-1)}{(n-1)}(2 + \frac{4(n-1)}{n})$$

$$\geq \left(\frac{2n+4n-4}{n}\right)$$

$$\geq \frac{2(3n-2)}{n}.$$

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