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Distinct Energies of Caffeine

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Abstract: The concept of energy of a graph was introduced by I. Gutman in the year 1978. In this article, we compute energy, Siedel energy, Distance energy, Harary energy, Maximum degree energy, Randić energy, Color energy and Laplacian energy of Caffeine.

Mathematics Subject Classification: 05C12, 05C90.

Keywords and Phrases: Eigenvalues, Energy, Siedel energy, Distance energy, Harary energy, Maximum degree energy, Randić energy, Color energy, Laplacian energy, Caffeine.

1. INTRODUCTION

Caffeine is a chemical found in coffee, tea, cola, guarana, mate, and other products. Caffeine is most commonly used to improve mental alertness, but it has many other uses. It is a central nervous system stimulant of the methylxanthine class. It is the world's most widely consumed psychoactive drug. It's molecular formula is $C_8H_{10}N_4O_2$. Its structure is shown in following figure-1.

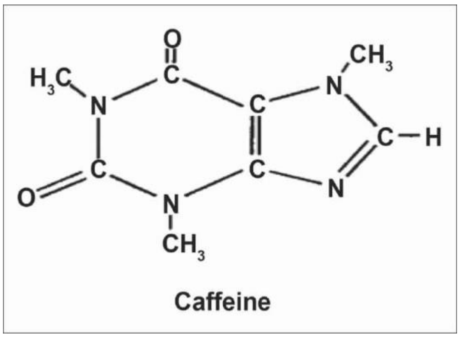
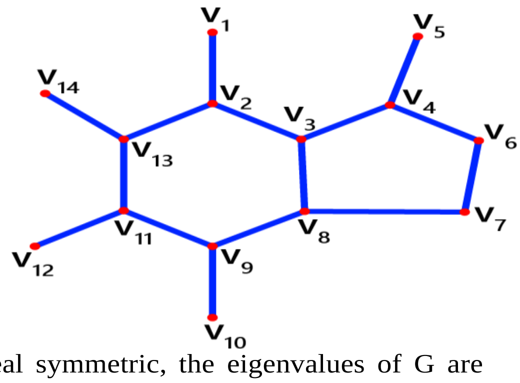


Figure-1

2 MAIN RESULTS

2.1 ENERGY OF A GRAPH

Study on energy of graphs goes back to the year 1978, when I. Gutman [12] defined this while working with energies of conjugated hydrocarbon containing carbon atoms. All graphs considered in this article are assumed to be simple without loops and multiple edges. Let $A = (a_{ij})$ be the adjacency matrix of the graph G with its eigenvalues $\rho_1, \rho_2, \rho_3, \ldots \rho_n$ assumed in decreasing order. Since A is



real symmetric, the eigenvalues of G are real numbers whose sum equal to zero. The sum of the absolute eigenvalues values of G is called the energy $\mathcal{E}(G)$ of G.

$$\text{i.e.,} \mathcal{E}(G) = \sum_{i=1}^{n} |\rho_i|.$$

Theories on the mathematical concepts of graph energy can be seen in the reviews [15], articles [14, 5, 6] and the references cited there in. For various upper and lower bounds for energy of a graph can be found in articles [17, 19] and it was observed that graph energy has chemical applications in the molecular orbital theory of conjugated molecules [13, 11].

Theorem 2.1. *The energy of Caffeine is 17.668.*

Proof: Consider a molecular graph of Caffeine as shown in the following figure-2. Here vertices are labeled from v_1 to v_{14}.

Figure-2

Adjacency matrix of Caffeine is,

$$A(C_8H_{10}N_4O_2) = \begin{array}{cc} & \begin{array}{cccccccccccccc} v_1 & v_2 & v_3 & v_4 & v_5 & v_6 & v_7 & v_8 & v_9 & v_{10} & v_{11} & v_{12} & v_{13} & v_{14} \end{array} \\ \begin{array}{c} v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \\ v_7 \\ v_8 \\ v_9 \\ v_{10} \\ v_{11} \\ v_{12} \\ v_{13} \\ v_{14} \end{array} & \left[\begin{array}{cccccccccccccc} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{array}\right] \end{array}$$

Characteristic equation is,
$$\rho^{14} - 15\rho^{12} + 82\rho^{10} - 2\rho^{9} - 205\rho^{8} + 14\rho^{7} + 238\rho^{6} - 28\rho^{5} - 116\rho^{4} + 14\rho^{3} + 21\rho^{2} - 2\rho - 1 = 0.$$

The eigenvalues of Caffeine are
$\rho_1 \approx -0.20608$, $\rho_2 \approx 0.35516$, $\rho_3 \approx -0.50286$, $\rho_4 \approx 0.48925$, $\rho_5 \approx 0.83155$, $\rho_6 \approx -0.7033$, $\rho_7 \approx -1.4354$, $\rho_8 \approx 1.104$, $\rho_9 \approx 1.9178$, $\rho_{10} \approx -1.6503$, $\rho_{11} \approx 2.505$, $\rho_{12} \approx 1.6314$, $\rho_{13} \approx -1.9084$ and $\rho_{14} \approx -2.4278$.

The energy of Caffeine is,
$\mathcal{E}(C_8H_{10}N_4O_2) = |-0.20608| + |0.35516| + |-0.50286| + |0.48925| + |0.83155| + |-0.7033| + |-1.4354| + |1.104| + |1.9178| + |-1.6503| + |2.505| + |1.6314| + |-1.9084| + |-2.4278|$.

$\therefore \mathcal{E}(C_8H_{10}N_4O_2) = 17.668.$

2.2 SEIDEL ENERGY

Let G be a simple graph of order n with vertex set $V = \{v_1, v_2, v_3, \ldots\ldots v_n\}$ and edge set E. The Seidel matrix of G is the $n \times n$ matrix defined by $S(G) := (s_{ij})$, where

$$s_{ij} = \begin{cases} -1, \text{if } v_iv_j \in E \\ 1 \text{ if } v_iv_j \notin E \\ 0 \text{ if } v_i = v_j. \end{cases}$$

The characteristic polynomial of S(G) is denoted by $f_n(G, \rho) = \det(\rho I - S(G))$. The Seidel eigenvalues of the graph G are the eigenvalues of S(G). Since S(G) is real and symmetric, its eigenvalues are real numbers. The Seidel energy [21] of G defined as $S\varepsilon(G) = \sum_{i=1}^{n} |\rho i|$.

Theorem2.2. *The Seidal energy of Caffeine is 40.485.*

Proof: The Seidel matrix of Caffeine is,

$$S(C_8H_{10}N_4O_2) = \begin{array}{cc} & \begin{array}{cccccccccccccc} v_1 & v_2 & v_3 & v_4 & v_5 & v_6 & v_7 & v_8 & v_9 & v_{10} & v_{11} & v_{12} & v_{13} & v_{14} \end{array} \\ \begin{array}{c} v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \\ v_7 \\ v_8 \\ v_9 \\ v_{10} \\ v_{11} \\ v_{12} \\ v_{13} \\ v_{14} \end{array} & \left[\begin{array}{cccccccccccccc} 0 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -1 & 0 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 1 \\ 1 & -1 & 0 & -1 & 1 & 1 & 1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & 0 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & -1 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & -1 & 1 & 0 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & -1 & 0 & -1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & 1 & 1 & 1 & -1 & 0 & -1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 0 & -1 & -1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 1 & 0 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 0 & 1 & 1 \\ 1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 1 & 0 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 0 \end{array}\right] \end{array}$$

The characteristic equation is,
$$\rho^{14} - 91\rho^{12} - 192\rho^{11} + 2109\rho^{10} + 6016\rho^{9} - 18239\rho^{8} - 63872\rho^{7} + 55187\rho^{6} + 279296\rho^{5} + 15263\rho^{4} - 443328\rho^{3} - 227345\rho^{2} + 66432\rho + 33851 = 0.$$

The Siedel eigenvalues of Caffeine are
$\rho_1 \approx 0.39663$, $\rho_2 \approx -0.35852$, $\rho_3 \approx -0.78302$, $\rho_4 \approx 1.8704$, $\rho_5 \approx -1.9476$, $\rho_6 \approx -2.0469$, $\rho_7 \approx -2.6632$, $\rho_8 \approx 2.2971$, $\rho_9 \approx 2.7743$, $\rho_{10} \approx -3.3415$, $\rho_{11} \approx 3.8495$, $\rho_{12} \approx -4.2632$, $\rho_{13} \approx -4.8385$ and $\rho_{14} \approx 9.0545$.

The Seidal energy of Caffeine is,
$S\mathcal{E}(C_8H_{10}N_4O_2) = |0.39663| + |-0.35852| + |-0.78302| + |1.8704| + |-1.9476| + |-2.0469| + |-2.6632| + |2.2971| + |2.7743| + |-3.3415| + |3.8495| + |-4.2632| + |-4.8385| + |9.0545|$.

$\therefore S\mathcal{E}(C_8H_{10}N_4O_2) = 40.485.$

2.3 DISTANCE ENERGY

On addressing problem for loop switching, R. L. Graham, H. O. Pollak [10] defined distance matrix of a graph. The concept of distance energy was defined by G. Indulal et al. [18] in the year 2008. Let G be a simple graph of order n with vertex set $V = \{v_1, v_2, ..., v_n\}$ and edge set E. Let d_{ij} be the distance between the vertices $v_i$and v_j then the $n \times n$ matrix $D(G) = (d_{ij})$ is called the distance matrix of G. The characteristic polynomial of D(G) is denoted by $f(G; \rho) = |\rho I - D(G)|$, where I is the unit matrix of order n. The roots $\rho_1, \rho_2, ..., \rho_n$ assumed in non-increasing order are called the distance eigenvalues of G. The distance energy of a graph G is defined as

$$D\varepsilon(G) = \sum_{i=1}^{n} |\rho_i|.$$

Since D(G) is a real symmetric matrix with zero trace, these distance eigenvalues are real with sum equal to zero.

Theorem2.3 *The Distance energy of Caffeine is 75.726.*

Proof: The Distance matrix of Caffeine is,

$$D(C_8H_{10}N_4O_2) = \begin{array}{cc} & \begin{array}{cccccccccccccc} v_1 & v_2 & v_3 & v_4 & v_5 & v_6 & v_7 & v_8 & v_9 & v_{10} & v_{11} & v_{12} & v_{13} & v_{14} \end{array} \\ \begin{array}{c} v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \\ v_7 \\ v_8 \\ v_9 \\ v_{10} \\ v_{11} \\ v_{12} \\ v_{13} \\ v_{14} \end{array} & \begin{bmatrix} 0 & 1 & 2 & 3 & 4 & 4 & 4 & 3 & 4 & 5 & 3 & 4 & 2 & 3 \\ 1 & 0 & 1 & 2 & 3 & 3 & 3 & 2 & 3 & 4 & 2 & 3 & 1 & 2 \\ 2 & 1 & 0 & 1 & 2 & 2 & 2 & 1 & 2 & 3 & 3 & 4 & 2 & 3 \\ 3 & 2 & 1 & 0 & 1 & 1 & 2 & 2 & 3 & 4 & 4 & 5 & 3 & 4 \\ 4 & 3 & 2 & 1 & 0 & 2 & 3 & 3 & 4 & 5 & 5 & 4 & 4 & 5 \\ 4 & 3 & 2 & 1 & 2 & 0 & 1 & 2 & 3 & 4 & 4 & 5 & 4 & 5 \\ 4 & 3 & 2 & 2 & 3 & 1 & 0 & 1 & 2 & 3 & 3 & 4 & 4 & 5 \\ 3 & 2 & 1 & 2 & 3 & 2 & 1 & 0 & 1 & 2 & 2 & 3 & 3 & 4 \\ 4 & 3 & 2 & 3 & 4 & 3 & 2 & 1 & 0 & 1 & 1 & 2 & 2 & 3 \\ 5 & 4 & 3 & 4 & 5 & 4 & 3 & 2 & 1 & 0 & 2 & 3 & 3 & 4 \\ 3 & 2 & 3 & 4 & 5 & 4 & 3 & 2 & 1 & 2 & 0 & 1 & 1 & 2 \\ 4 & 3 & 4 & 5 & 6 & 5 & 4 & 3 & 2 & 3 & 1 & 0 & 2 & 3 \\ 2 & 1 & 2 & 3 & 4 & 4 & 4 & 3 & 2 & 3 & 1 & 2 & 0 & 1 \\ 3 & 2 & 3 & 4 & 5 & 5 & 5 & 4 & 3 & 4 & 2 & 3 & 1 & 0 \end{bmatrix} \end{array}$$

Characteristic equation is,
$\rho^{14} - 872\rho^{12} - 16934\rho^{11} - 144322\rho^{10} - 686010\rho^9 - 1990505\rho^8 - 3665696\rho^7 - 4327488\rho^6 - 3227680\rho^5 - 1453120\rho^4 - 356096\rho^3 - 36096\rho = 0.$

Distance eigenvalues Caffeine are
$\rho_1 \approx 0.0$, $\rho_2 \approx 0.0$, $\rho_3 \approx -0.35595$, $\rho_4 \approx -0.45445$, $\rho_5 \approx -0.75793$, $\rho_6 \approx -1.035$, $\rho_7 \approx -1.1806$, $\rho_8 \approx -1.8473$, $\rho_9 \approx -2.2021$, $\rho_{10} \approx -3.1745$, $\rho_{11} \approx -3.8735$, $\rho_{12} \approx -9.2955$, $\rho_{13} \approx -13.686$ and $\rho_{14} \approx 37.863$.

Distance energy of Caffeine is,
$D\mathcal{E}(C_8H_{10}N_4O_2) = |\,0.0\,| + |\,0.0\,| + |-0.35595| + |-0.45445| + |-0.75793| + |-1.035| + |-1.1806| + |-1.8473| + |-2.2021| + |-3.1745| + |-3.8735| + |-9.2955| + |-13.686| + |37.863|.$

$\therefore D\mathcal{E}(C_8H_{10}N_4O_2) = 75.726.$

2.4 HARARY ENERGY

The concept of Harary energy was introduced by A.Dilek Güngör and A.SinanÇevik [8]. The Harary matrix of G is the square matrix of order n whose (i, j)-entry is$\frac{1}{dij}$ where d_{ij} between the vertices v_i and v_j. Let $\rho_1, \rho_2, ..., \rho_n$ be the eigenvalues of the Harary matrix of G. The Harary energy, $H\mathcal{E}(G)$ is defined by

$$H\varepsilon(G) = \sum_{i=1}^{n} |\rho_i|.$$

Further studies on Harary energy can be found in [22].

Theorem 2.4 *The Harary energy of Caffeine is 17.45*

Proof: The Harary matrix of Caffeine is,

Harary eigenvalues of Caffeine are
$\rho_1 \approx -0.06114$, $\rho_2 \approx -0.20823$, $\rho_3 \approx 0.18343$, $\rho_4 \approx -0.40737$, $\rho_5 \approx -0.71092$, $\rho_6 \approx -0.81789$, $\rho_7 \approx -0.96032$, $\rho_8 \approx 0.96864$, $\rho_9 \approx -1.2803$, $\rho_{10} \approx -1.366$, $\rho_{11} \approx -1.5023$, $\rho_{12} \approx 1.5037$, $\rho_{13} \approx -1.4103$ and $\rho_{14} \approx 6.069$.

Harary energy of Caffeine is,
$H\mathcal{E}(C_8H_{10}N_4O_2) = |-0.06114| + |-0.20823| + |0.18343| + |-0.40737| + |-0.71092| + |-0.81789| + |-0.96032| + |0.96864| + |-1.2803| + |-1.366| + |-1.5023| + |1.5037| + |-1.4103| + |6.069|.$

$\therefore H\mathcal{E}(C_8H_{10}N_4O_2) = 17.45.$

2.5 MAXIMUM DEGREE ENERGY

In the year 2009 C. Adiga and M. Smitha [1] defined maximum degree energy of a graph. Let G be a simple graph of order n with vertex set $V=\{v_1,v_2,....v_n\}$ and edge set E. The maximum degree matrix of G is the $n \times n$ matrix defined by $A_{MD}(G) = (a_{ij})$, where

$$L_{ij} = \begin{cases} \max[d(v_i), d(v_j)] & \text{if } v_iv_j \in E \\ 0 & \text{otherwise} \end{cases}$$

The characteristic polynomial of $A_{MD}(G)$ is denoted by $f_n(G, \rho) = \det(\rho I - A_{MD}(G))$. The maximum degree eigenvalues of the graph Gare the eigenvalues of $A_{MD}(G)$. Since $A_{MD}(G)$ real and symmetric, its eigenvalues are real numbers and we label them in non-increasing order$\rho_1\rho_{2,\ldots,}\rho_n$.The maximum degree energy of G is defined as,

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

Theorem 2.5 *The Maximum degree energy of Caffeine is 50.292*.

Proof: The Maximum degree matrix of Caffeine is,

$$MD(C_8H_{10}N_4O_2) = \begin{array}{cc} & \begin{matrix} v_1 & v_2 & v_3 & v_4 & v_5 & v_6 & v_7 & v_8 & v_9 & v_{10} & v_{11} & v_{12} & v_{13} & v_{14} \end{matrix} \\ \begin{matrix} v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \\ v_7 \\ v_8 \\ v_9 \\ v_{10} \\ v_{11} \\ v_{12} \\ v_{13} \\ v_{14} \end{matrix} & \begin{bmatrix} 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 3 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 3 & 0 & 3 & 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 3 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 & 0 & 3 & 0 & 3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 & 0 & 3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 \end{bmatrix} \end{array}$$

Characteristic equation is,
$\rho^{14} - 121\rho^{12} + 5337\rho^{10} - 324\rho^{9} - 107649\rho^{8} + 17496\rho^{7} + 1021329\rho^{6} - 262440\rho^{5} - 4297455\rho^{4} + 1417176\rho^{3} + 6790635\rho^{2} - 2125764\rho - 2125764 = 0$.

$$H(C_8H_{10}N_4O_2) = \begin{array}{cc} & \begin{matrix} v_1 & v_2 & v_3 & v_4 & v_5 & v_6 & v_7 & v_8 & v_9 & v_{10} & v_{11} & v_{12} & v_{13} & v_{14} \end{matrix} \\ \begin{matrix} v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \\ v_7 \\ v_8 \\ v_9 \\ v_{10} \\ v_{11} \\ v_{12} \\ v_{13} \\ v_{14} \end{matrix} & \begin{bmatrix} 0 & 1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \frac{1}{3} & \frac{1}{4} & \frac{1}{2} & \frac{1}{3} \\ 1 & 0 & 1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{2} & \frac{1}{3} & 1 & \frac{1}{2} \\ \frac{1}{2} & 1 & 0 & 1 & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{3} & \frac{1}{4} & \frac{1}{2} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{2} & 1 & 0 & 1 & 1 & \frac{1}{2} & \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{4} & \frac{1}{5} & \frac{1}{3} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{3} & \frac{1}{2} & 1 & 0 & \frac{1}{2} & \frac{1}{3} & \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \frac{1}{5} & \frac{1}{4} & \frac{1}{4} & \frac{1}{5} \\ \frac{1}{4} & \frac{1}{3} & \frac{1}{2} & 1 & \frac{1}{2} & 0 & 1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{4} & \frac{1}{5} & \frac{1}{4} & \frac{1}{5} \\ \frac{1}{4} & \frac{1}{3} & \frac{1}{2} & \frac{1}{2} & \frac{1}{3} & 1 & 0 & 1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{3} & \frac{1}{4} & \frac{1}{4} & \frac{1}{5} \\ \frac{1}{3} & \frac{1}{2} & 1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{2} & 1 & 0 & 1 & \frac{1}{2} & \frac{1}{2} & \frac{1}{3} & \frac{1}{3} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{3} & \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{3} & \frac{1}{2} & 1 & 0 & 1 & 1 & \frac{1}{2} & \frac{1}{2} & \frac{1}{3} \\ \frac{1}{5} & \frac{1}{4} & \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \frac{1}{4} & \frac{1}{3} & \frac{1}{2} & 1 & 0 & \frac{1}{2} & \frac{1}{3} & \frac{1}{3} & \frac{1}{4} \\ \frac{1}{3} & \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \frac{1}{4} & \frac{1}{3} & \frac{1}{2} & 1 & \frac{1}{2} & 0 & 1 & 1 & \frac{1}{2} \\ \frac{1}{4} & \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \frac{1}{6} & \frac{1}{5} & \frac{1}{4} & \frac{1}{3} & \frac{1}{2} & \frac{1}{3} & 1 & 0 & \frac{1}{2} & \frac{1}{3} \\ \frac{1}{2} & 1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{3} & \frac{1}{2} & \frac{1}{3} & 1 & \frac{1}{2} & 0 & 1 \\ \frac{1}{3} & \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{4} & \frac{1}{3} & \frac{1}{4} & \frac{1}{2} & \frac{1}{3} & 1 & 0 \end{bmatrix} \end{array}$$

Maximum degree eigenvalues are
$\rho_1 \approx -0.46444$, $\rho_2 \approx 0.89234$, $\rho_3 \approx -1.6097$, $\rho_4 \approx 1.732$, $\rho_5 \approx 2.0986$, $\rho_6 \approx -2.4042$, $\rho_7 \approx -3.3073$, $\rho_8 \approx 3.3792$, $\rho_9 \approx 4.3373$, $\rho_{10} \approx -5.0594$, $\rho_{11} \approx -5.4352$, $\rho_{12} \approx 5.6317$, $\rho_{13} \approx -6.8657$ and $\rho_{14} \approx 7.0747$.

The maximum degree energy of Caffeine is,
$MD\mathcal{E}(C_8H_{10}N_4O_2) = |-0.46444| + |0.89234| + |-1.6097| + |1.732| + |2.0986| + |-2.4042| + |-3.3073| + |3.3792| + |4.3373| + |-5.0594| + |-5.4352| + |5.6317| + |-6.8657| + |7.0747|$.

$\therefore MD\mathcal{E}(C_8H_{10}N_4O_2) = 50.292$.

2.6 RANDIĆ ENERGY

It was in the year 1975, Milan Randić invented a molecular structure descriptor called Randić index which is defined as [20]

$$R(G) = \sum_{v_iv_j \in E(G)} \frac{1}{\sqrt{d_i d_j}}.$$

Motivated by this S.B.Bozkurt et al. [3] defined Randić matrix and Randić energy as follows. Let G be graph of order n with vertex set $V=\{v_1,v_2,\ldots,v_n\}$ and edge set E. Randic matrix of G is a $n \times n$ symmetric matrix defined by $R(G) := (r_{ij})$,

$$\text{Where } r_{ij} = \begin{cases} \frac{1}{\sqrt{d_i d_j}} & \text{if } v_iv_j \in E(G) \\ 0 & \text{otherwise} \end{cases}$$

The characteristic equation of R(G) is defined by $f_n(G, \rho) = \det(\rho I\ R(G)) = 0$. The roots of this equation are called Randić eigenvalues of G. Since R(G) is real and symmetric, its eigenvalue sare real numbers and we label them indecreasing order $\rho_1 \geq \rho_2 \geq \ldots \geq \rho_n$. Randić energy of G is defined as,

$$R\mathcal{E}(G) = \sum_{i=1}^{n} |\rho_i|$$

Further studies on Randić energy can be seen in the articles [4, 9, 7] and the references cited there in.

Theorem2.6. *The Randić energy of Caffeine is 8.4077.*

Proof: The Randić matrix of Caffeine is,

$$R(C_8H_{10}N_4O_2)=\begin{array}{c@{}c} & \begin{array}{cccccccccccccc} v_1 & v_2 & v_3 & v_4 & v_5 & v_6 & v_7 & v_8 & v_9 & v_{10} & v_{11} & v_{12} & v_{13} & v_{14} \end{array} \\ \begin{array}{c} v_1\\ v_2\\ v_3\\ v_4\\ v_5\\ v_6\\ v_7\\ v_8\\ v_9\\ v_{10}\\ v_{11}\\ v_{12}\\ v_{13}\\ v_{14} \end{array} & \begin{bmatrix}
0 & \frac{1}{\sqrt{3}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{\sqrt{3}} & 0 & \frac{1}{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{1}{3} & 0 & \frac{1}{3} & 0 & 0 & 0 & \frac{1}{3} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \frac{1}{3} & 0 & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{6}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{1}{\sqrt{3}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{2} & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \frac{1}{3} & 0 & 0 & 0 & \frac{1}{\sqrt{6}} & 0 & \frac{1}{3} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{3} & 0 & \frac{1}{\sqrt{3}} & \frac{1}{3} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{3}} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{3} & 0 & 0 & \frac{1}{\sqrt{3}} & \frac{1}{3} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{3}} & 0 & 0 & 0 \\
0 & \frac{1}{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{3} & 0 & 0 & \frac{1}{\sqrt{3}} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{3}} & 0
\end{bmatrix} \end{array}$$

Randić eigenvalues of Caffeine are
$\rho_1 \approx -0.13462$, $\rho_2 \approx 0.1918$, $\rho_3 \approx -0.37673$, $\rho_4 \approx 0.36976$, $\rho_5 \approx 0.4619$, $\rho_6 \approx -0.44906$, $\rho_7 \approx -0.72572$, $\rho_8 \approx 0.56934$, $\rho_9 \approx 0.75125$, $\rho_{10} \approx -0.68938$, $\rho_{11} \approx -0.96825$, $\rho_{12} \approx 0.85981$, $\rho_{13} \approx -0.8601$ and $\rho_{14} \approx 1.0$.

Randić energy of Caffeine is,
$R\mathcal{E}(C_8H_{10}N_4O_2) = |-0.13462| + |0.1918| + |-0.37673| + |0.36976| + |0.4619| + |-0.44906| + |-0.72572| + |0.56934| + |0.75125| + |-0.68938| + |-0.96825| + |0.85981| + |-0.8601| + |1.0|$.

$\therefore R\mathcal{E}(C_8H_{10}N_4O_2) = 8.4077$.

2.7. COLOR ENERGY

Let G be a simple graph of order n with vertex set $V = \{v_1, v_2, ..., v_n\}$ and edge set E. The color matrix of G is the $n \times n$ matrix defined by $A_c(G) := (a_{ij})$,

$$a_{ij} = \begin{cases} 1, & \text{if } v_i \text{and} v_j \text{are adjacent with } C(v_i) \neq C(V_j) \\ -1 & \text{if } v_i \text{and} v_j \text{are non adjacent with } C(v_i) = C(V_j) \\ 0 & \text{otherwise} \end{cases}$$

The characteristic polynomial of $A_c(G)$ is denoted by $f_n(G, \rho) = \det(\rho I - A_c(G))$. If the color used is minimum then the adjacency matrix is denoted by $A_\chi(G)$. The eigenvalues of the graph G, its eigenvalues are real numbers and we label them in non–increasing order $\rho_1 \geq \rho_2 \geq \ldots \geq_{,n}$. The color energy [2] of G is defined as,

$$C\mathcal{E}(G) = \sum_{I=1}^{n} |\rho_i|$$

If the color used is minimum then the energy is called chromatic energy and it is denoted by $\mathcal{E}_\chi(G)$.

Theorem 2.7. *The chromatic energy of Caffeine is 27.342.*

Proof: The vertices $V_1, V_2, V_3, V_4, V_5, V_6, V_7, V_8, V_9, V_{10}, V_{11}, V_{12}, V_{13}$ and V_{14} of Caffeine are colored by minimum colors A, B, A, B, A, A, C, B, A, B, B, A, A and B respectively. Chromatic matrix of Caffeine is,

$$C(C_8H_{10}N_4O_2)=\begin{array}{c@{}c} & \begin{array}{cccccccccccccc} v_1 & v_2 & v_3 & v_4 & v_5 & v_6 & v_7 & v_8 & v_9 & v_{10} & v_{11} & v_{12} & v_{13} & v_{14} \end{array} \\ \begin{array}{c} v_1\\ v_2\\ v_3\\ v_4\\ v_5\\ v_6\\ v_7\\ v_8\\ v_9\\ v_{10}\\ v_{11}\\ v_{12}\\ v_{13}\\ v_{14} \end{array} & \begin{bmatrix}
0 & 1 & -1 & 0 & -1 & -1 & 0 & 0 & -1 & 0 & 0 & -1 & -1 & 0 \\
1 & 0 & 1 & -1 & 0 & 0 & 0 & -1 & 0 & -1 & -1 & 0 & 1 & -1 \\
-1 & 1 & 0 & 1 & -1 & -1 & 0 & 1 & -1 & 0 & 0 & -1 & -1 & 0 \\
0 & -1 & 1 & 0 & 1 & 1 & 0 & -1 & 0 & -1 & -1 & 0 & 0 & -1 \\
-1 & 0 & -1 & 1 & 0 & -1 & 0 & 0 & -1 & 0 & 0 & -1 & -1 & 0 \\
-1 & 0 & -1 & 1 & -1 & 0 & 1 & 0 & -1 & 0 & 0 & -1 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 1 & -1 & 0 & 0 & 1 & 0 & 1 & -1 & -1 & 0 & 0 & -1 \\
-1 & 0 & -1 & 0 & -1 & -1 & 0 & 1 & 0 & 1 & 1 & -1 & -1 & 0 \\
0 & -1 & 0 & -1 & 0 & 0 & 0 & -1 & 1 & 0 & -1 & 0 & 0 & -1 \\
0 & -1 & 0 & -1 & 0 & 0 & 0 & -1 & 1 & -1 & 0 & 1 & 1 & -1 \\
-1 & 0 & -1 & 0 & -1 & -1 & 0 & 0 & -1 & 0 & 1 & 0 & -1 & 0 \\
-1 & 1 & -1 & -1 & 0 & -1 & 0 & 0 & -1 & 0 & 1 & -1 & 0 & 1 \\
0 & -1 & 0 & 0 & -1 & 0 & 0 & -1 & 0 & -1 & -1 & 0 & 1 & 0
\end{bmatrix} \end{array}$$

Characteristic equation is,
$\rho^{14} - 51\rho^{12} + 148\rho^{11} + 349\rho^{10} - 2178\rho^9 + 2913\rho^8 + 1106\rho^7 - 5375\rho^6 + 2574\rho^5 + 2348\rho^4 - 2056\rho^3 - 76\rho^2 + 352\rho - 52 = 0$.

Chromatic eigenvalues of Caffeine are
$\rho_1 \approx 0.18169$, $\rho_2 \approx -0.50069$, $\rho_3 \approx 0.65416$, $\rho_4 \approx 0.82839$, $\rho_5 \approx 1.276$, $\rho_6 \approx -0.75367$, $\rho_7 \approx -0.97904$, $\rho_8 \approx 1.4647$, $\rho_9 \approx 1.65$, $\rho_{10} \approx 2.1577$, $\rho_{11} \approx 2.5917$, $\rho_{12} \approx 2.8668$, $\rho_{13} \approx -3.7723$ and $\rho_{14} \approx -7.6654$.

Chromatic energy of Caffeine is,
$C\mathcal{E}(C_8H_{10}N_4O_2) = |0.18169| + |-0.50069| + |0.65416| + |0.82839| + |1.276| + |-0.75367| + |-0.97904| + |1.4647| + |1.65| + |2.1577|\ 2.5917| + |2.8668| + |-3.7723| + |-7.6654|$.

$\therefore C\mathcal{E}(C_8H_{10}N_4O_2) = 27.342$.

2.8. LAPLACIAN ENERGY

I.Gutman and B. Zhou [16] defined the Laplacian energy of a graph G in the year 2006. Let G be a graph with n vertices and m edges. The Laplacian matrix of the graph G, denoted by $L = (L_{ij})$, is a square matrix of order n whose elements are defined as,

$$L_{ij} = \begin{cases} -1, & \text{if } v_i \text{and} v_j \text{are adjacent} \\ 1 & \text{if } v_i \text{and} v_j \text{are non adjacent} \\ 0 & \text{if } i = j \end{cases}$$

Where d_i is the degree of the vertex v_i. Let be the Laplacian eigenvalues of G. Laplacian energy $L\mathcal{E}(G)$ of G is defined as

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

Theorem 2.8. *Laplacian energy of caffeine is 20.969.*

Proof: Degree Matrix Caffeine is,

$$D(C_8H_{10}N_2O_2) = \begin{array}{cc} & \begin{array}{cccccccccccccc} v_1 & v_2 & v_3 & v_4 & v_5 & v_6 & v_7 & v_8 & v_9 & v_{10} & v_{11} & v_{12} & v_{13} & v_{14} \end{array} \\ \begin{array}{c} v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \\ v_7 \\ v_8 \\ v_9 \\ v_{10} \\ v_{11} \\ v_{12} \\ v_{13} \\ v_{14} \end{array} & \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \end{array}$$

Adjacency matrix of Caffeine is,

$$A(C_8H_{10}N_4O_2) = \begin{array}{cc} & \begin{array}{cccccccccccccc} v_1 & v_2 & v_3 & v_4 & v_5 & v_6 & v_7 & v_8 & v_9 & v_{10} & v_{11} & v_{12} & v_{13} & v_{14} \end{array} \\ \begin{array}{c} v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \\ v_7 \\ v_8 \\ v_9 \\ v_{10} \\ v_{11} \\ v_{12} \\ v_{13} \\ v_{14} \end{array} & \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix} \end{array}$$

Laplacian matrix of Caffeine is,

$L\mathcal{E}(C_8H_{10}N_4O_2) = D(C_8H_{10}N_4O_2) - A(C_8H_{10}N_4O_2)$

$$L(C_8H_{10}N_4O_2) = \begin{array}{cc} & \begin{array}{cccccccccccccc} v_1 & v_2 & v_3 & v_4 & v_5 & v_6 & v_7 & v_8 & v_9 & v_{10} & v_{11} & v_{12} & v_{13} & v_{14} \end{array} \\ \begin{array}{c} v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \\ v_7 \\ v_8 \\ v_9 \\ v_{10} \\ v_{11} \\ v_{12} \\ v_{13} \\ v_{14} \end{array} & \begin{bmatrix} 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 3 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & -1 & 3 & -1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 3 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 2 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 2 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & -1 & 3 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 3 & -1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 3 & -1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 3 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 \end{bmatrix} \end{array}$$

Characteristic equation is,
$\rho 14 - 30\rho 13 + 397 \rho 12 - 3056 \rho 11 + 15199 \rho 10 - 51324 \rho 9 + 120427 \rho 8 - 197712 \rho 7 + 225883 \rho 6 - 176506 \rho 5 + 91339 \rho 4 - 29552 \rho 3 + 5342 \rho 2 - 406 \rho = 0.$

Laplacian eigenvalues are
$\rho_1 = 0.0$, $\rho_2 = 0.2604$, $\rho_3 = 0.41397$, $\rho_4 = 0.61766$, $\rho_5 = 0.73432$, $\rho_6 = 0.84225$, $\rho_7 = 1.694$, $\rho_8 = 2.0958$, $\rho_9 = 2.3947$, $\rho_{10} = 2.8101$, $\rho_{11} = 3.9102$, $\rho_{12} = 4.3622$, $\rho_{13} = 4.5679$ and $\rho_{14} = 5.2966$.

Number of vertices = 14 and Number of edges = 15
Average degree $= \frac{2m}{n} = \frac{2\times 15}{14} = \frac{15}{7} = 2.1429$
Laplacian energy of Caffeine is,

$L\mathcal{E}(C_8H_{10}N_4O_2) = |0.0-2.1429|+|0.2604-2.1429|+0.41397-2.1429|+|0,61766-2.1429|+0.73432-2.1429|+|0.84225-2.1429|+1.694-2.1429|+|2.0958-2.1429|+|2.3947-2.1429|+|2.8101-2.1429|+ |3.9102-2.1429|+|3.9102-2.1429|+|4.3622-2.1429|+|4.5679-2.1429|+|5.2966-2.1429|.$

$L\mathcal{E}(C_8H_{10}N_4O_2) = |-2.1429|+|-1.8825|+|-1.7289| +|-1.5252|+|-1.4085|+|-1.3006|+|-0.44886|+ |-.047057|+|0.25184|+|0.66724|+|1.7673|+|2.2193| +|2.425| +|3.1537|.$

$L\mathcal{E}(C_8H_{10}N_4O_2) = 20.969$

3. CONCLUSION

In this article, we compute Energy, Siedel energy, Distance energy, Harary energy, Maximum degree energy, Randić energy, Color energy and Laplacian energy of Caffeine.

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