DISTINCT ENERGIES OF NICOTINE

[1]H.L.PARASHIVAMURTHY, [2]M.R.RAJESH KANNA, [3]R.JAGADEESH
[1,2,3]Assistant professor
[1]Research Scholar,Research and Development Centre,
Bharathiar University, Coimbatore- 641 046, India.
[1]BGS Institute of Technology, Adichunchanagiri University, B.G. Nagar-571448,
Nagamangala Taluk, Mandya District, India.
[2]Department of Mathematics,Sri.D Devaraja Urs Governement First Grade College,
Hunsur - 571 105 ,India.
[3]Government Science College (Autonomous),
Nrupathunga Road, Bangalore - 560 001, India.

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

Mathematics Subject Classification: 05C12, 05C90.

Keywords and Phrases: Eigenvalues, Energy, Siedel energy, Distance energy, Harary energy, Maximum degree energy, Randiŝ energy, Laplacian energy.

1 Introduction

Nicotine is a chemical that contains nitrogen, which is made by several types of plants, including the tobacco plant. It is also produced synthetically. Its molecular formula is $C_{10}H_{14}N_2$.

2 Main Results

2.1 Energy of agraph

Study on energy of graphs goes back to the year 1978, when I. Gutman [13] de- fined this while working with energies of conjugated hydrocarbons containing car- bon 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 eigen values $\lambda_1, \lambda_2, \lambda_3, , \lambda_n$ assumed in non increasing order. Since A is real symmetric, the eigenvalues of Gare real numbers whose sum equal to zero. The sum of the absolute eigenvalues of G is called the energy E (G) of G.
i.e., $\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda i|$

Theories on the mathematical concepts of graph energy can be seen in the reviews [17], articles [16, 6, 7] and the references cited there in. For various upper and lower bounds for energy of a graph can be found in articles [18, 20] and it was observed that graph energy has chemical applications in the molecular orbital theory of conjugated molecules [15, 12].

Theorem 2.1. The energy of Nicotine is 15.88877914.
Proof. Consider a molecular graph of $C_{10}H_{14}N_2$ as shown in the following Fig. Here vertices are numbered from v_1 to v_{12}.

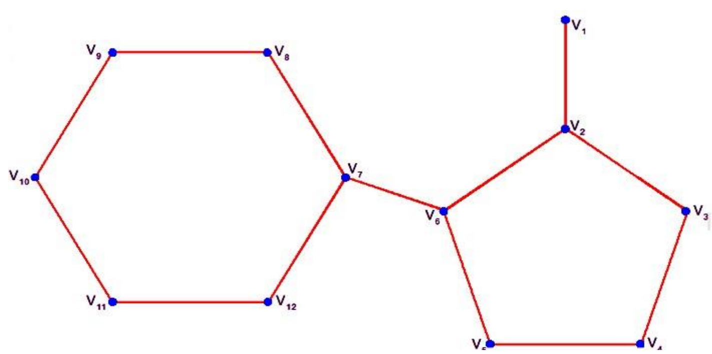

Figure: Molecular Graph ($\mathbf{C_{10}H_{14}N_2}$)

Adjacency matrix is,

$A(C_{10}H_{14}N_2) = $

	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_1	0	1	0	0	0	0	0	0	0	0	0	0
V_2	1	0	1	0	0	1	0	0	0	0	0	0
V_3	0	1	0	1	0	0	0	0	0	0	0	0
V_4	0	0	1	0	1	0	0	0	0	0	0	0
V_5	0	0	0	1	0	1	0	0	0	0	0	0
V_6	0	1	0	0	1	0	1	0	0	0	0	0
V_7	0	0	0	0	0	1	0	1	0	0	0	1
V_8	0	0	0	0	0	0	1	0	1	0	0	0
V_9	0	0	0	0	0	0	0	1	0	1	0	0
V_{10}	0	0	0	0	0	0	0	0	1	0	1	0
V_{11}	0	0	0	0	0	0	0	0	0	1	0	1
V_{12}	0	0	0	0	0	0	1	0	0	0	1	0

Characteristic equation is,
$\lambda^{12} - 13\lambda^{10} + 61\lambda^8 - 2\lambda^7 - 129\lambda^6 + 12\lambda^5 + 126\lambda^4 - 18\lambda^3 - 50\lambda^2 + 8\lambda + 4 = 0.$

The Eigenvalues are
$\lambda_1 \approx -2.253271607$, $\lambda_2 \approx -1.8136606504$, $\lambda_3 \approx -1.644850338$, $\lambda_4 \approx -1.000000$, $\lambda_5 \approx -0.99999999$, $\lambda_6 \approx -0.2326611251$, $\lambda_7 \approx 0.4706834214$, $\lambda_8 \approx 0.999999999$, $\lambda_9 \approx 1.0000000$, $\lambda_{10} \approx 1.203312890$, $\lambda_{11} \approx 1.927470184$ and $\lambda_{12} \approx 2.342923083$.

The energy of Nicotine is,
$E(C_{10}H_{14}N_2) = |-2.253271607| + |-1.8136606504| + |-1.644850338| + |-1.000000| + |-0.99999999| + |-0.2326611251| + |0.4706834214| + |0.999999999| + |1.0000000| + |1.203312890| + |1.927470184| + |2.342923083|.$

$\therefore \varepsilon(C_{10}H_{14}N_2) = 15.88877914.$

2.2. Seidel 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 Seidel matrix of G is the n × n matrix defined by $S(G) := (s_{ij})$, where

$$Sij = \begin{cases} -1, \text{if } vivj \in E \\ 1 \text{ if } vivj \notin E \\ 0 \text{ if } vi = vj. \end{cases}$$

The characteristic polynomial of S(G) is denoted by $f_n(G, \lambda) = \det(\lambda I - S(G))$. 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 [22] of G defined as $S\varepsilon(G) = \sum_{i=1}^{n} |\lambda i|$.

Theorem 2.2. The Seidal energy of Nicotine is 34.37038021.
Proof. The Seidal matrix of Nicotine is,

$$S(C_{10}H_{14}N_2) = \begin{bmatrix} & V_1 & V_2 & V_3 & V_4 & V_5 & V_6 & V_7 & V_8 & V_9 & V_{10} & V_{11} & V_{12} \\ V_1 & 0 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ V_2 & -1 & 0 & -1 & 1 & 1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 \\ V_3 & 1 & -1 & 0 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ V_4 & 1 & 1 & -1 & 0 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ V_5 & 1 & 1 & 1 & -1 & 0 & -1 & 1 & 1 & 1 & 1 & 1 & 1 \\ V_6 & 1 & -1 & 1 & 1 & -1 & 0 & -1 & 1 & 1 & 1 & 1 & 1 \\ V_7 & 1 & 1 & 1 & 1 & 1 & -1 & 0 & -1 & 1 & 1 & 1 & -1 \\ V_8 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 0 & -1 & 1 & 1 & 1 \\ V_9 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 0 & -1 & 1 & 1 \\ V_{10} & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 0 & -1 & 1 \\ V_{11} & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 0 & -1 \\ V_{12} & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 1 & 1 & 1 & -1 & 0 \end{bmatrix} -$$

Characteristic equation is,

$\lambda^{12} - 66\lambda^{10} - 56\lambda^9 + 1347\lambda^8 + 1344\lambda^7 - 11820\lambda^6 - 10096\lambda^5 + 47479\lambda^4 + 25088\lambda^3 - 77362\lambda^2 - 8088\lambda + 32229 = 0.$

Siedel Eigen values are

$\lambda_1 \approx -4.882298713$, $\lambda_2 \approx -3.610300917$, $\lambda_3 \approx -3.000000000$, $\lambda_4 \approx -2.999999999$, $\lambda_5 \approx -1.950079570$, $\lambda_6 \approx -0.7425109118$, $\lambda_7 \approx 0.999999999$, $\lambda_8 \approx 1.000000001$, $\lambda_9 \approx 2.270740644$, $\lambda_{10} \approx 2.600322274$, $\lambda_{11} \approx 3.473881337$ and $\lambda_{12} \approx 6.840245853$.

The Seidal energy of Nicotine is,

$E(C_{10}H_{14}N_2) = |-4.882298713| + |-3.610300917| + |-3.000000000| + |-2.999999999| + |-1.950079570| + |-0.7425109118| + |0.999999999| + |1.000000001| + |2.270740644| + |2.600322274| + |3.473881337| + |6.840245853|$.

$\therefore S\varepsilon(C_{10}H_{14}N_2) = 34.37038021$.

2.3. Distance energy of a graph

On addressing problem for loop switching, R. L. Graham, H. O. Pollak [11] defined distance matrix of a graph. The concept of distance energy was defined by G. Indulal et al. [19] 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 $f(G;\lambda) = |\lambda I - D(G)|$, where I is the unit matrix of order n. The roots $\lambda_1, \lambda_2, ..., \lambda_n$ assumed in non increasing order are called the distance eigenvalues of G. The distance energy of a graph G is n defined as $D\varepsilon(G) = \sum_{i=1}^{n} |\lambda i|$.

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

Theorem 2.3. The Distance energy of Nicotine is 65.34918301.

Proof. The Distance matrix of Nicotine is, D ($C_{10}H_{14}N_2$) =

	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_1	0	1	2	3	3	2	3	4	5	6	5	4
V_2	1	0	1	2	2	1	2	3	4	5	4	3
V_3	2	1	0	1	2	2	3	4	5	6	5	4
V_4	3	2	1	0	1	2	3	4	5	6	5	4
V_5	3	2	2	1	0	1	2	3	4	5	4	3
V_6	2	1	2	2	1	0	1	2	3	4	3	2
V_7	3	2	3	3	2	1	0	1	2	3	2	1
V_8	4	3	3	4	3	2	1	0	1	2	3	2
V_9	5	4	5	5	4	3	2	1	0	1	2	3
V_{10}	6	5	6	6	5	4	3	2	1	0	1	2
V_{11}	5	4	5	5	5	3	2	3	2	1	0	1
V_{12}	4	3	4	4	3	2	1	2	3	2	1	0

Characteristic equation is,
$\lambda^{12}-691\lambda^{10}-10160\lambda^{9}-63362\lambda^{8}-208796\lambda^{7}-386607\lambda^{6}-405040\lambda^{5}-231780\lambda^{4}-65568\lambda^{3}-7104\lambda^{2}=0.$

Distance eigenvalues are
$\lambda_1\approx32.67459146$, $\lambda_2\approx-16.13487836$, $\lambda_3\approx-4.209428768$, $\lambda_4\approx-3.99999999995$, $\lambda_5\approx-3.864090773$, $\lambda_6\approx-1.737937829$, $\lambda_7\approx-1.167281680$, $\lambda_8\approx-0.8757231664$, $\lambda_9\approx-0.3141062787$, $\lambda_{10}\approx-0.3711446917$, $\lambda_{11}\approx-0.000071351$ and $\lambda_{12}\approx$
-0.0000269053.

Distance energy of Nicotine is,
$D\varepsilon$ ($C_{10}H_{14}N_2$) = | 32.67459146 | + | −16.13487836 | + | −4.209428768 | + |−3.9999999999 |+ |−3.864090773 |+ |−1.737937829 |+ | −1.167281680 |+ |−0.8757231664 |+ |−0.3141062787 |+ |−0.3711446917 |+ |−0.000071351 |+ | −0.0000269053 |.

∴ $D\varepsilon$ (D)($C_{10}H_{14}N_2$)= 65.34918301.

2.4. Harary energy of a graph

The concept of Harary energy was introduced by A. Dilek Güngör and A. Sinan Çevik [9]. The Harary matrix of G is the square matrix of order n whose (i, j)-^{n}1 entry is $\frac{1}{dij}$ Where dij is the distance between the vertices vi and vj let λ1, λ2, λ3…, λn be the eigenvalues of the Harary matrix of G. The Harary energy, HE(G) is defined by $H\varepsilon(G)=\sum_{i=1}^{n}|\lambda i|$. Further studies on Harary energy can be found in [23].

Theorem 2.4. The Harary energy of Nicotine is 15.14784691.

Proof. The Harary matrix of Nicotine is,

$$
H\,(C_{10}H_{14}N_2) = \left[\begin{array}{ccccccccccccc}
 & V_1 & V_2 & V_3 & V_4 & V_5 & V_6 & V_7 & V_8 & V_9 & V_{10} & V_{11} & V_{12} \\
V_1 & 0 & 1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{3} & \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \frac{1}{6} & \frac{1}{5} & \frac{1}{4} \\
V_2 & 1 & 0 & 1 & \frac{1}{2} & \frac{1}{2} & 1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \frac{1}{4} & \frac{1}{3} \\
V_3 & \frac{1}{2} & 1 & 0 & 1 & \frac{1}{2} & \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \frac{1}{6} & \frac{1}{5} & \frac{1}{4} \\
V_4 & \frac{1}{3} & \frac{1}{2} & 1 & 0 & 1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \frac{1}{6} & \frac{1}{5} & \frac{1}{4} \\
V_5 & \frac{1}{3} & \frac{1}{2} & \frac{1}{2} & 1 & 0 & 1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \frac{1}{4} & \frac{1}{3} \\
V_6 & \frac{1}{2} & 1 & \frac{1}{2} & \frac{1}{2} & 1 & 0 & 1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{3} & \frac{1}{2} \\
V_7 & \frac{1}{3} & \frac{1}{2} & \frac{1}{3} & \frac{1}{3} & \frac{1}{2} & 1 & 0 & 1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{2} & 1 \\
V_8 & \frac{1}{4} & \frac{1}{3} & \frac{1}{3} & \frac{1}{4} & \frac{1}{3} & \frac{1}{2} & 1 & 0 & 1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{2} \\
V_9 & \frac{1}{5} & \frac{1}{4} & \frac{1}{5} & \frac{1}{5} & \frac{1}{4} & \frac{1}{3} & \frac{1}{2} & 1 & 0 & 1 & \frac{1}{2} & \frac{1}{3} \\
V_{10} & \frac{1}{6} & \frac{1}{5} & \frac{1}{6} & \frac{1}{6} & \frac{1}{5} & \frac{1}{4} & \frac{1}{3} & \frac{1}{2} & 1 & 0 & 1 & \frac{1}{2} \\
V_{11} & \frac{1}{5} & \frac{1}{4} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{3} & \frac{1}{2} & \frac{1}{3} & \frac{1}{2} & 1 & 0 & 1 \\
V_{12} & \frac{1}{4} & \frac{1}{3} & \frac{1}{4} & \frac{1}{4} & \frac{1}{3} & \frac{1}{2} & 1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{2} & 1 & 0
\end{array}\right]
$$

Characteristic equation is,

$$\lambda^{12} - \frac{71657}{3600}\lambda^{10} - \frac{100289}{2160}\lambda^{9} + \frac{5631967}{1296000}\lambda^{8} + \frac{25616201}{2160000}\lambda^{7} + \frac{273082080941}{1866240000}\lambda^{6} + \frac{32572005737}{622080000}\lambda^{5}$$

$$-\frac{1036157965978}{671846400000}\lambda^{4} - \frac{4305115089373}{403107840000}\lambda^{3} - \frac{66087665839}{7558270000}\lambda^{2} + \frac{561974702021}{967458816000}\lambda - \frac{1016440741337}{14511882240000} = 0$$

Harary eigenvalues are

$\lambda_1 \approx 5.263307388$, $\lambda_2 \approx 1.700670654$, $\lambda_3 \approx 0.2648735021$, $\lambda_4 \approx 0.1784052538$, $\lambda_5 \approx 0.1666666687$, $\lambda_6 \approx -0.3842094189$, $\lambda_7 \approx -0.7358015718$, $\lambda_8 \approx -1.470000465$, $\lambda_9 \approx -1.354066613$, $\lambda_{10} \approx -1.290072503$, $\lambda_{11} \approx -1.166666668$ and $\lambda_{12} \approx -1.173106211$.

Harary energy of Nicotine is,

$H\varepsilon\,(C_{10}H_{14}N_2) = |5.263307388| + |1.700670654| + |0.2648735021| + |0.1784052538| + |0.1666666687| + |-0.3842094189| + |-0.7358015718| + |-1.47000465| + |-1.354066613| + |-1.290072503| + |-1.166666668| + |-1.173106211|$.

$\therefore H\mathcal{E}\,(C_{10}H_{14}N_2) = 15.14784691$.

2.5 Maximum degree energy of a graph

In the year 2009 Prof. 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 $V = \{v_1, v_2 \ldots v_n\}$ and edge set E. The maximum degree matrix of G is the n × n matrix defined by The characteristic polynomial of $A_{MD}(G)$ is denoted by $f_n(G, \lambda) = \det(\lambda I - A_{MD}(G))$. The maximum degree eigenvalues of the graph G are the eigenvalues of $A_{MD}(G)$. Since $A_{MD}(G)$ is real and symmetric, its eigenvalues are real numbers and we label them in non-increasing order $\lambda_1, \lambda_2, \cdots, \lambda_n$. The maximum degree energy of G is defined as $MD\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda i|$.

Theorem2. 5. The maximum degree energy of Nicotine is 39.14085174.

Proof. The maximum degree matrix of Nicotine is,

$A_{MD}(C_{10}H_{14}N_2)$ =

	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_1	0	3	0	0	0	0	0	0	0	0	0	0
V_2	3	0	3	0	0	3	0	0	0	0	0	0
V_3	0	3	0	2	0	0	0	0	0	0	0	0
V_4	0	0	2	0	2	0	0	0	0	0	0	0
V_5	0	0	0	2	0	3	0	0	0	0	0	0
V_6	0	3	0	0	3	0	3	0	0	0	0	0
V_7	0	0	0	0	0	3	0	3	0	0	0	2
V_8	0	0	0	0	0	0	3	0	2	0	0	0
V_9	0	0	0	0	0	0	0	2	0	2	0	0
V_{10}	0	0	0	0	0	0	0	0	2	0	2	0
V_{11}	0	0	0	0	0	0	0	0	0	2	0	2
V_{12}	0	0	0	0	0	0	3	0	0	0	2	0

Characteristic equation is,

$$\lambda^{12} - 84\lambda^{10} + 2348\,\lambda^8 - 216\,\lambda^7 - 27702\,\lambda^6 + 6696\,\lambda^5 + 1441\,\lambda^4 - 49248\,\lambda^3 - 301968\,\lambda^2 + 103680\,\lambda + 155520 = 0\,.$$

Maximum degree eigenvalues are

$\lambda_1 \approx -6.37869526$, $\lambda_2 \approx 6.546458290$, $\lambda_3 \approx -4.591381895$, $\lambda_4 \approx 4.603782541$, $\lambda_5 \approx -3.611337810$, $\lambda_6 \approx -0.6400733821$, λ_7 2.906828153, $\lambda_8 \approx 1.213502871$, $\lambda_9 \approx 2.299854018$, $\lambda_{10} \approx -2.348937530$, $\lambda_{11} \approx 2.000000000$ and $\lambda_{12} \approx -1.999999999$.

The maximum degree energy of Nicotine is,

$MD\varepsilon\,(C_{10}H_{14}N_2) = |-6.37869526| + |6.546458290| + |-4.591381895| + |4.603782541| + |-3.611337810| + |-0.6400733821| + |2.906828153| + |1.213502871| + |2.299854018| + |-2.348937530| + |2.0000000| + |-1.99999999|$.

$\therefore MD\varepsilon\,(C_{10}H_{14}N_2) = 39.14085174$.

2.6 Randić energy of a graph

It was in the year 1975, Milan Randić invented a molecular structure descriptor called Randić index which is defined as [21]

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

Motivated by this S.B.Bozkurt et al.[4] defined Randić matrix and Randić energy as follows. Let G be graph of order n with vertex set $V = \{v_1, v_2, ..., v_n\}$ and edge set E. Randić matrix of G is a $n \times n$ symmetric matrix defined by $R(G) := (r_{ij})$,

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

The characteristic equation of R(G) is defined by $f_n(G, \lambda) = \det(\lambda I \ R(G)) = 0$. The roots of this equation is called Randić eigenvalues of G. Since R(G) is real and symmetric, its eigenvalues are real numbers and we label them in decreasing order $\lambda_1 \geq, \lambda_2 \geq, \lambda_3 \geq \ldots, \geq \lambda_n$. Randi'c energy of G if difined as $R\varepsilon(G) = \sum_{i=1}^{n} |\lambda i|$. Further studies on Randić energy can be seen in the articles [5, 10, 8] and the references cited there in.

Theorem 2.6. The Randić energy of Nicotine is 7.38731432.

Proof. The Randić matrix of Nicotine is,

$$
R\,(C_{10}H_{14}N_2) = \begin{bmatrix}
 & V_1 & V_2 & V_3 & V_4 & V_5 & V_6 & V_7 & V_8 & V_9 & V_{10} & V_{11} & V_{12} \\
V_1 & 0 & \frac{1}{\sqrt{3}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
V_2 & \frac{1}{\sqrt{3}} & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & \frac{1}{3} & 0 & 0 & 0 & 0 & 0 & 0 \\
V_3 & 0 & \frac{1}{\sqrt{6}} & 0 & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
V_4 & 0 & 0 & \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
V_5 & 0 & 0 & 0 & \frac{1}{2} & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & 0 & 0 & 0 & 0 \\
V_6 & 0 & \frac{1}{3} & 0 & 0 & \frac{1}{\sqrt{6}} & 0 & \frac{1}{3} & 0 & 0 & 0 & 0 & 0 \\
V_7 & 0 & 0 & 0 & 0 & 0 & \frac{1}{3} & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & 0 & \frac{1}{\sqrt{6}} \\
V_8 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{6}} & 0 & \frac{1}{2} & 0 & 0 & 0 \\
V_9 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\
V_{10} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & 0 & \frac{1}{2} & 0 \\
V_{11} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & 0 & \frac{1}{2} \\
V_{12} & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & 0 & \frac{1}{2} & 0
\end{bmatrix}
$$

Characteristic equation is,

$$\lambda^{12} - \frac{49}{18}\lambda^{10} + \frac{1189}{432}\lambda^{8} - \frac{1}{36}\lambda^{7} - \frac{371}{288}\lambda^{6} + \frac{1}{27}\lambda^{5} + \frac{247}{864}\lambda^{4} - \frac{7}{576}\lambda^{3} - \frac{27}{576}\lambda^{2} + \frac{1}{864}\lambda + \frac{1}{1728} = 0.$$

Randić eigenvalues are

$\lambda_1 \approx -0.9739968365$, $\lambda_2 \approx -0.8466074193$, $\lambda_3 \approx -0.7705862713$, $\lambda_4 \approx -0.500000003$, $\lambda_5 \approx -0.4573067450$, $\lambda_6 \approx -0.1451598440$, $\lambda_7 \approx 0.2115445800$, $\lambda_8 \approx 0.5165865656$, $\lambda_9 \approx 0.5463086012$, $\lambda_{10} \approx 0.9192173695$, $\lambda_{11} \approx 0.500000000$ and $\lambda_{12} \approx 1.000000000$.

Randić energy of Nicotine is,

$R\varepsilon\,(C_{10}H_{14}N_2) = |-0.9739968365| + |-0.8466074193| + |-0.7705862713| + |-0.50000003| + |-0.4573067450| + |-0.1451598440| + |0.2115445800| + |0.5165865656| + |0.5463086012| + |0.9192173695| + |0.5000000| + |1.0000000|$.

$\therefore R\varepsilon\,(C_{10}H_{14}N_2) = 7.38731432$.

2.7 Laplacian energy of a graph

I. Gutman and B. Zhou [14] 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

$$\mathrm{Lij} = \begin{cases} -1 \text{ if vi and vj are adjacent} \\ 0 \text{ if vi and vj are not adjacent} \\ \text{di if } i = j \end{cases}$$

where d_i is the degree of the vertex v_i. Let $\mu_1, \mu_2, \cdots, \mu_n$ be the Laplacian eigen Values of G, Laplacian energy LE(G) of G Defined as $D\varepsilon(G) = \sum_{i=1}^{n} \left|\mu i - \frac{2m}{n}\right|$.

Theorem 2. 7. The Laplacian energy of Nicotine is 16.67194076.

Proof. The Laplacian Degree matrix of Nicotine is,

$$D\,(C_{10}H_{14}N_2) = \begin{bmatrix} & V_1 & V_2 & V_3 & V_4 & V_5 & V_6 & V_7 & V_8 & V_9 & V_{10} & V_{11} & V_{12} \\ V_1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ V_2 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ V_3 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ V_4 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ V_5 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ V_6 & 0 & 0 & 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ V_7 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 \\ V_8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ V_9 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ V_{10} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 \\ V_{11} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 \\ V_{12} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 \end{bmatrix}$$

Adjacency matrix of energy is,

$$A\,(C_{10}H_{14}N_2) = \begin{bmatrix} & V_1 & V_2 & V_3 & V_4 & V_5 & V_6 & V_7 & V_8 & V_9 & V_{10} & V_{11} & V_{12} \\ V_1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ V_2 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ V_3 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ V_4 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ V_5 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ V_6 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ V_7 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 1 \\ V_8 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ V_9 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ V_{10} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ V_{11} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ V_{12} & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

The Laplacian matrix of Nicotine is,

$LA_{(C10H14N2)} = D_{(C10H14N2)} - A_{(C10H14N2)}$

=

	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_1	1	−1	0	0	0	0	0	0	0	0	0	0
v_2	−1	3	−1	0	0	−1	0	0	0	0	0	0
v_3	0	−1	2	−1	0	0	0	0	0	0	0	0
v_4	0	0	−1	2	−1	0	0	0	0	0	0	0
v_5	0	0	0	−1	2	−1	0	0	0	0	0	0
v_6	0	−1	0	0	−1	3	−1	0	0	0	0	0
v_7	0	0	0	0	0	−1	3	−1	0	0	0	−1
v_8	0	0	0	0	0	0	−1	2	−1	0	0	0
v_9	0	0	0	0	0	0	0	−1	2	−1	0	0
v_{10}	0	0	0	0	0	0	0	0	−1	2	−1	0
v_{11}	0	0	0	0	0	0	0	0	0	−1	2	−1
v_{12}	0	0	0	0	0	0	−1	0	0	0	−1	2

Characteristic equation is,
$\lambda^{12} + 26\lambda^{11} + 295\lambda^{10} + 1920\lambda^9 + 7925\lambda^8 + 21652\lambda^7 + 39662\lambda^6 + 48254\lambda^5 + 37712\lambda^4+17652\lambda^3 + 4269\lambda^2 + 360\lambda = 0.$

Number of vertices = 12 and Number of edges = 13.

$\therefore$Averge degree $= \frac{2m}{n} = \frac{2\times13}{12} = \frac{13}{6} = 2.166666667.$

Laplacian eigenvalues are
$\lambda_1 \approx 0.0$, $\lambda_2 \approx 0.1626431234$, $\lambda_3 \approx 0.7026219332$, $\lambda_4 \approx 1.0$, $\lambda_5 \approx 1.12713145$, $\lambda_6 \approx 1.671633113$, $\lambda_7 \approx 2.206275553$, $\lambda_8 \approx 3.0$, $\lambda_9 \approx 3.276010468$, $\lambda_{10} \approx 3.750972704$, $\lambda_{11} \approx 4.154043169$ and $\lambda_{12} \approx 4.948668486$.

Laplacian energy of Nicotine is,
$L\varepsilon\ (C_{10}H_{14}N_2)$ = | 0.0-2.166666667 | + | 0.1626431234-2.166666667 | + |0.7026219332 −2.166666667 | + |1.0-2.166666667 | + | 1.12713145-2.166666667 | + | 1.671633113-2.166666667 | + |2.206275553-2.166666667 |+ |3.0-2.166666667 | + | 3.276010468-2.166666667 | + |3.750972704-2.166666667 | + |4.154043169-2.166666667 | + |4.948668486-2.166666667 |.

$L\varepsilon\ (C_{10}H_{14}N_2)$ = | −2.166666667 | + | −2.004023543 | + | −1.464044733 | + |−1.166666667 | + | −1.039535217 | + | −0.4950335537 | + | 0.03960888633 |+ | 0.8333333333 | + | 1.109343801 | + | 1.584306037 | + | 1.987376502 | + | 2.782001819 |.

$\therefore L\varepsilon\ (C_{10}H_{14}N_2) = 16.67194076.$

Conclusion:

In this article, we compute energy, Siedel energy, distance energy, Harary energy, maximum degree energy, Randić energy and Laplacian energy of Nicotine.

References

[1] C. Adiga and M. Smitha, On maximum degree energy of a graph. Int. J. Con- temp. Math. Sciences, Vol. **4**, no. 8, (2009), 385 - 396.

[2] C.Adiga, E. Sampathkumar, M.A. Sriraj, Shrikanth A. S, Color Energy of a Graph Jangjeon Mathematical Society, 16(2013), No. 3, 335 - 351.

[3] Bales, JR; Nicholson JK; Sadler PJ (1985). ”Two-dimensional proton nuclear magnetic resonance ”maps” of acetaminophen metabolites in human urine”. Clin- ical Chemistry. 31 (5): 757-762. PMID 3987005. Archived from the original on 2008-11-21.

[4] S. B. Bozkurt, A. D. Güngör and I. Gutman, Randić spectral radius and Randić energy, Commun. Math. Comput. Chem, **64** (2010) 239-250.

[5] S. B. Bozkurt and D. Bozkurt, Sharp Upper Bounds for Energy and Randić Energy, Commun. Math. Comput. Chem, **70** (2013) 669-680.

[6] D. Cvetković and I. Gutman (eds.), Applications of Graph Spectra (Mathematical Institution, Belgrade, 2009).

[7] D. Cvetković and I. Gutman (eds.), Selected Topics on Applications of Graph Spectra, (Mathematical Institute Belgrade, 2011).

[8] K. C. Das, Sezer Sorgun and I. Gutman, On Randić Energy, Commun. Math. Comput. Chem, **73** (2015) 81-92.

[9] A. Dilek Güngör, A. Sinan Çevik, On the Harary Energy and Harary Estrada Index of a Graph MATCH Commun. Math. Comput. Chem. **64** (2010) 281-296.

[10] A. Dilek Maden, New Bounds on the Incidence Energy, Randić Energy and Randić Estrada Index, Commun. Math. Comput. Chem, **74** (2015) 367-387.

[11] R. L. Graham and H. O. Pollak. On the addressing problem for loop switching. Bell Labs Technical Journal, **50**, (1971), 2495-2519.

[12] A. Graovac, I. Gutman and N. Trinajstić, Topological Approach to the Chem- istry of Conjugated Molecules (Springer, Berlin), (1977).

[13] I. Gutman, The energy of a graph. it Ber. Math-Statist. Sekt. Forschungsz. Graz, **103**, (1978), 1-22.

[14] I. Gutman and B. Zhou, Laplacian energy of a graph. Lin. Algebra Appl. **414**, 29 - 37 (2006).

[15] I. Gutman and O. E. Polansky, Mathematical Concepts in Organic Chemistry (Springer, Berlin), (1986).

[16] I. Gutman, The energy of a graph: Old and New Results,ed.by A. Betten, A. Kohnert, R. Laue, A. Wassermann. Algebraic Combinatorics and Applications (Springer, Berlin), (2001), pp. 196 - 211.

[17] I. Gutman, X. Li and J. Zhang, in Graph Energy,ed. by M. Dehmer, F. Emmert- Streib. it Analysis of Complex Networks. From Biology to Linguistics(Wiley - VCH, Weinheim), (2009), pp. 145-174.

[18] Huiqing Liu, Mei Lu and Feng Tian, Some upper bounds for the energy of graphs Journal of Mathematical Chemistry, Vol. **41**, No.1, (2007).

[19] G. Indulal, I. Gutman, and A. Vijayakumar. On distance energy of graphs. MATCH Communications in Mathematical and in Computer Chemistry, **60**, (2008), 461-472.

[20] B. J. McClelland, Properties of the latent roots of a matrix: The estimation of π-electron energies. J. Chem. Phys., **54**, (1971), 640 - 643.

[21] M. Randić, On Characterization of molecular branching, J. Amer. Chem. Soc., **97**, (1975), 6609-6615.

[22] Willem H. Haemers, Seidel Switching and Graph Energy, MATH Commun. Math. Comput. Chem, **68** (2012), 653-659.

[23] Zhihui Cui, Bolian Liu, On Harary Matrix, Harary Index and Harary Energy, MATCH Commun. Math. Comput. Chem. **68** (2012) 815-823.

* * * * * * * * * *