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Distinct Energies of Paracetamol

M. R. Rajesh Kanna[1,*] and R. Jagadeesh[2,3]

1 Department of Mathematics, Sri D.Devaraja Urs Government First Grade College, Hunsur, Karnataka, India.

2 Department of Mathematics, Government Science College (Autonomous), N.T.Road, Bangalore, Karnataka, India.

3 Department of Mathematics, Government First Grade College, Ramanagara, Karnataka, 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 Color energy of Paracetamol.

MSC: 05C12, 05C90.

Keywords: Eigenvalues, Energy, Siedel Energy, Distance Energy, Harary Energy, Maximum Degree Energy, Randić Energy, Color Energy, Paracetamol graph.

1. Introduction

Paracetamol also known as acetaminophen or APAP is a medication used to treat pain and fever. It is typically used for mild to moderate pain. Paracetamol is used to treat many conditions such as headache, muscle aches, arthritis, backache, toothaches, colds and fevers. Paracetamol was discovered in 1877 [20]. It is on the World Health Organization's List of Essential Medicines, the most effective and safe medicines needed in a health system [23]. Paracetamol is available as a generic medication with trade names including Tylenol and Panadol among others [17]. Paracetamol consists of a benzene ring core, substituted by one hydroxyl group and the nitrogen atom of an amide group in the para $(1,4)$ pattern [3]. The amide group is acetamide (ethanamide). It is an extensively conjugated system, as the lone pair on the hydroxyl oxygen, the benzene pi cloud, the nitrogen lone pair, the p orbital on the carbonyl carbon, and the lone pair on the carbonyl oxygen are all conjugated. The presence of two activating groups also make the benzene ring highly reactive toward electrophilic aromatic substitution. It's molecular formula is $C_8H_9NO_2$

2. Energy of a Graph

Study on energy of graphs goes back to the year 1978, when I. Gutman [13] 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 $\rho_1, \rho_2, \rho_3, \cdots, \rho_n$ 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. i.e., $\mathcal{E}(G) = \sum_{i=1}^{n} |\rho_i|$.

* *E-mail: mr.rajeshkanna@gmail.com*

Theories on the mathematical concepts of graph energy can be seen in the reviews [16], articles [6, 7, 15] and the references cited there in. For various upper and lower bounds for energy of a graph can be found in articles [18, 21] and it was observed that graph energy has chemical applications in the molecular orbital theory of conjugated molecules [12, 14].

Theorem 2.1. *The energy of paracetamol* $\mathcal{E}(C_8H_9NO_2) = 13 \cdot 22162$

Proof. Consider a molecular graph of paracetamol $C_8H_9NO_2$ as shown in the following figure−1. Here vertices are numbered from v_1 to v_{11}.

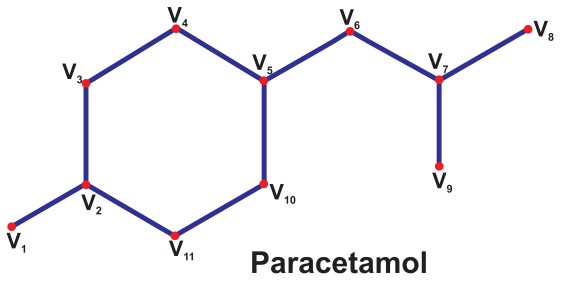

Figure 1.

Adjacency matrix of paracetamol is

$$A(C_8H_9NO_2) = \begin{array}{c|ccccccccccc} & v_1 & v_2 & v_3 & v_4 & v_5 & v_6 & v_7 & v_8 & v_9 & v_{10} & v_{11} \\ \hline v_1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ v_2 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ v_3 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ v_4 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ v_5 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ v_6 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ v_7 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 \\ v_8 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ v_9 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ v_{10} & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ v_{11} & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{array}$$

Characteristic equation is

$$\rho^{11} - 11\rho^9 + 41\rho^7 - 61\rho^5 + 32\rho^3 - 2\rho = 0.$$

Eigenvalues are $\rho_1 \approx 0$, $\rho_2 \approx -0.26811$, $\rho_3 \approx 0.26811$, $\rho_4 \approx -1.0$, $\rho_5 \approx 1.0000$, $\rho_6 \approx 1.3125$, $\rho_7 \approx -1.3125$, $\rho_8 \approx -1.8103$, $\rho_9 \approx 1.8103$, $\rho_{10} \approx 2.2199$ and $\rho_{11} \approx -2.2199$. The energy of paracetamol

$$\mathcal{E}(C_8H_9NO_2) = | 0 | + | -0.26811 | + | 0.26811 | + | -1.0 | + | 1.0 | + | 1.3125 | + | -1.3125 | + | -1.8103 | + | 1.8103 | + | 2.2199 | + | -2.2199 | .$$

The energy of paracetamol is, $\mathcal{E}(C_8H_9NO_2) = 13 \cdot 22162$. □

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

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

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 [24] of G defined as

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

Theorem 3.1. *The Seidal energy of paracetamol is,* $S\mathcal{E}(C_8H_9NO_2) = 29 \cdot 22026$.

Proof. Siedel matrix of paracetamol is

$$S(C_8H_9NO_2) = \left(\begin{array}{c|cccccccccccc} & v_1 & v_2 & v_3 & v_4 & v_5 & v_6 & v_7 & v_8 & v_9 & v_{10} & v_{11} \\ \hline v_1 & 0 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ v_2 & -1 & 0 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 \\ v_3 & 1 & -1 & 0 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ v_4 & 1 & 1 & -1 & 0 & -1 & 1 & 1 & 1 & 1 & 1 & 1 \\ v_5 & 1 & 1 & 1 & -1 & 0 & -1 & 1 & 1 & 1 & -1 & 1 \\ v_6 & 1 & 1 & 1 & 1 & -1 & 0 & -1 & 1 & 1 & 1 & 1 \\ v_7 & 1 & 1 & 1 & 1 & 1 & -1 & 0 & -1 & -1 & 1 & 1 \\ v_8 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 0 & 1 & 1 & 1 \\ v_9 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 1 & 0 & 1 & 1 \\ v_{10} & 1 & 1 & 1 & 1 & -1 & 1 & 1 & 1 & 1 & 0 & -1 \\ v_{11} & 1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 0 \end{array}\right)$$

Characteristic equation is

$$\rho^{11} - 55\rho^9 - 46\rho^8 + 850\rho^7 + 824\rho^6 - 4790\rho^5 - 3988\rho^4 + 9805\rho^3 + 7224\rho^2 - 5811\rho - 4014 = 0$$

Siedel eigenvalues are $\rho_1 \approx -0.65486$, $\rho_2 \approx -1.0$, $\rho_3 \approx 1.0$, $\rho_4 \approx 1.6053$, $\rho_5 \approx -1.548$, $\rho_6 \approx -3.0$, $\rho_7 \approx 2.1284$, $\rho_8 \approx 3.4261$, $\rho_9 \approx -3.7668$, $\rho_{10} \approx -4.6405$ and $\rho_{11} \approx 6.4503$. The Seidal energy of paracetamol

$$\begin{aligned} S\mathcal{E}(C_8H_9NO_2) =& \mid -0.65486 \mid + \mid -1.0 \mid + \mid 1.0 \mid + \mid 1.6053 \mid + \mid -1.5480 \mid + \mid -3.0 \mid + \mid 2.1284 \mid + \mid 3.4261 \mid + \mid -3.7668 \mid \\ & + \mid -4.6405 \mid + \mid 6.4503 \mid \end{aligned}$$

The Seidal energy of paracetamol is, $S\mathcal{E}(C_8H_9NO_2) = 29 \cdot 22026$. □

4. Distance Energy

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 $f(G;\rho) = |\rho I - D(G)|$, 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

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

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

Theorem 4.1. *The Distance energy of paracetamol is,* $D\mathcal{E}(C_8H_9NO_2) = 62 \cdot 97956$.

Proof. Distance matrix of paracetamol is,

$$D(C_8H_9NO_2) = \left(\begin{array}{c|cccccccccc} & v_1 & v_2 & v_3 & v_4 & v_5 & v_6 & v_7 & v_8 & v_9 & v_{10} & v_{11} \\ \hline v_1 & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 7 & 3 & 2 \\ v_2 & 1 & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 6 & 2 & 1 \\ v_3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 5 & 5 & 3 & 2 \\ v_4 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 4 & 2 & 3 \\ v_5 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 3 & 1 & 2 \\ v_6 & 5 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 2 & 2 & 3 \\ v_7 & 7 & 5 & 4 & 3 & 2 & 1 & 0 & 1 & 1 & 3 & 4 \\ v_8 & 8 & 6 & 5 & 4 & 3 & 2 & 1 & 0 & 2 & 4 & 5 \\ v_9 & 8 & 6 & 5 & 4 & 3 & 2 & 1 & 2 & 0 & 4 & 5 \\ v_{10} & 3 & 2 & 3 & 2 & 1 & 2 & 3 & 4 & 4 & 0 & 1 \\ v_{11} & 2 & 1 & 2 & 3 & 2 & 3 & 4 & 5 & 5 & 1 & 0 \end{array}\right)$$

Characteristic equation is

$$\rho^{11} - 650\rho^9 - 8560\rho^8 - 46372\rho^7 - 129604\rho^6 - 200280\rho^5 - 169680\rho^4 - 69184\rho^3 - 4800\rho^2 + 4864\rho + 1024 = 0$$

Distance eigenvalues are $\rho_1 \approx 0.24867$, $\rho_2 \approx -0.33941$, $\rho_3 \approx -0.50519$, $\rho_4 \approx -0.88961$, $\rho_5 \approx -0.98978$, $\rho_6 \approx -1.3832$, $\rho_7 \approx -2.0$, $\rho_8 \approx -4.1356$, $\rho_9 \approx -4.5781$, $\rho_{10} \approx -16.669$ and $\rho_{11} \approx 31.241$. Distance energy of paracetamol is,

$$\begin{aligned} D\mathcal{E}(C_8H_9NO_2) =& \mid 0.24867 \mid + \mid -0.33941 \mid + \mid -0.50519 \mid + \mid -0.88961 \mid + \mid -0.98978 \mid + \mid -1.3832 \mid + \mid -2.0 \mid \\ & + \mid -4.1356 \mid + \mid -4.5781 \mid + \mid -16.669 \mid + \mid 31.241 \mid \end{aligned}$$

Distance energy of paracetamol $D\mathcal{E}(C_8H_9NO_2) = 62 \cdot 97956$. □

5. Harary Energy

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)-entry is $\frac{1}{d_{ij}}$ where d_{ij} is the distance between the vertices v_i and v_j . Let $\rho_1, \rho_2, \ldots, \rho_n$ be the eigenvalues of the Harary matrix of G. The Harary energy, $H\mathcal{E}(G)$ is defined by

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

Further studies on Harary energy can be found in [25].

Theorem 5.1. *The Harary energy of paracetamol* $H\mathcal{E}(C_8H_9NO_2) = 13 \cdot 81697$

Proof. Harary matrix of paracetamol is,

$$H(C_8H_9NO_2) = \left(\begin{array}{c|ccccccccccc} & v_1 & v_2 & v_3 & v_4 & v_5 & v_6 & v_7 & v_8 & v_9 & v_{10} & v_{11} \\ \hline v_1 & 0 & 1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \frac{1}{6} & \frac{1}{7} & \frac{1}{7} & \frac{1}{3} & \frac{1}{2} \\ v_2 & 1 & 0 & 1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \frac{1}{6} & \frac{1}{6} & \frac{1}{2} & 1 \\ v_3 & \frac{1}{2} & 1 & 0 & 1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \frac{1}{5} & \frac{1}{3} & \frac{1}{2} \\ v_4 & \frac{1}{3} & \frac{1}{2} & 1 & 0 & 1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{4} & \frac{1}{2} & \frac{1}{3} \\ v_5 & \frac{1}{4} & \frac{1}{3} & \frac{1}{2} & 1 & 0 & 1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{3} & 1 & \frac{1}{2} \\ v_6 & \frac{1}{5} & \frac{1}{4} & \frac{1}{3} & \frac{1}{2} & 1 & 0 & 1 & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{3} \\ v_7 & \frac{1}{7} & \frac{1}{5} & \frac{1}{4} & \frac{1}{3} & \frac{1}{2} & 1 & 0 & 1 & 1 & \frac{1}{3} & \frac{1}{4} \\ v_8 & \frac{1}{8} & \frac{1}{6} & \frac{1}{5} & \frac{1}{4} & \frac{1}{3} & \frac{1}{2} & 1 & 0 & \frac{1}{2} & \frac{1}{4} & \frac{1}{5} \\ v_9 & \frac{1}{8} & \frac{1}{6} & \frac{1}{5} & \frac{1}{4} & \frac{1}{3} & \frac{1}{2} & 1 & \frac{1}{2} & 0 & \frac{1}{4} & \frac{1}{5} \\ v_{10} & \frac{1}{3} & \frac{1}{2} & \frac{1}{3} & \frac{1}{2} & 1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{4} & 0 & 1 \\ v_{11} & \frac{1}{2} & 1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \frac{1}{5} & 1 & 0 \end{array}\right)$$

Harary eigenvalues are $\rho_1 \approx 0.16682$, $\rho_2 \approx -0.48665$, $\rho_3 \approx -0.50345$, $\rho_4 \approx 0.41482$, $\rho_5 \approx -0.73743$, $\rho_6 \approx -1.1666$, $\rho_7 \approx -1.2388$, $\rho_8 \approx 1.5587$, $\rho_9 \approx -1.3514$, $\rho_{10} \approx -1.4242$ and $\rho_{11} \approx 4.7681$. Harary energy of paracetamol

$$\begin{aligned} H\mathcal{E}(C_8H_9NO_2) =& \mid 0.16682 \mid + \mid -0.48665 \mid + \mid -0.50345 \mid + \mid 0.41482 \mid + \mid -0.73743 \mid + \mid -1.1666 \mid + \mid -1.2388 \mid \\ & + \mid 1.5587 \mid + \mid -1.3514 \mid + \mid -1.4242 \mid + \mid 4.7681 \mid \end{aligned}$$

The Harary energy of paracetamol $H\mathcal{E}(C_8H_9NO_2) = 13 \cdot 81697$. □

6. Maximum Degree Energy

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 $V = \{v_1, v_2, ...v_n\}$ and edge set E. The maximum degree matrix of G is the $n \times n$ matrix defined by $A_{MD}(G) = (a_{ij})$, where

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

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 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 $\rho_1 \geqslant \rho_2 \geqslant \cdots \geqslant \rho_n$. The maximum degree energy of G is defined as $MD\mathcal{E}(G) = \sum_{i=1}^{n} |\rho_i|$.

Theorem 6.1. *The maximum degree energy of paracetamol is,* $MD\mathcal{E}(C_8H_9NO_2) = 36 \cdot 52702$

Proof. Maximum degree matrix of paracetamol is,

$$A_{MD}(C_8H_9NO_2) = \left(\begin{array}{c|ccccccccccc} & v_1 & v_2 & v_3 & v_4 & v_5 & v_6 & v_7 & v_8 & v_9 & v_{10} & v_{11} \\ \hline v_1 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ v_2 & 3 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 \\ v_3 & 0 & 3 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ v_4 & 0 & 0 & 2 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ v_5 & 0 & 0 & 0 & 3 & 0 & 3 & 0 & 0 & 0 & 3 & 0 \\ v_6 & 0 & 0 & 0 & 0 & 3 & 0 & 3 & 0 & 0 & 0 & 0 \\ v_7 & 0 & 0 & 0 & 0 & 0 & 3 & 0 & 3 & 3 & 0 & 0 \\ v_8 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 \\ v_9 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 \\ v_{10} & 0 & 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 2 \\ v_{11} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 \end{array}\right)$$

Characteristic equation is

$$\rho^{11} - 89\rho^9 + 2626\rho^7 - 28584\rho^5 + 83592\rho^3 - 23328\rho = 0$$

Maximum degree eigenvalues are $\rho_1 = 0$, $\rho_2 \approx 0.55791$, $\rho_3 \approx -0.55791$, $\rho_4 \approx -2.0$, $\rho_5 \approx 2.0$, $\rho_6 \approx 4.0695$, $\rho_7 \approx -4.0695$, $\rho_8 \approx -5.3555$, $\rho_9 \approx 5.3555$, $\rho_{10} \approx 6.2806$ and $\rho_{11} \approx -6.2806$. The maximum degree energy of paracetamol is,

$$\begin{aligned} MD\mathcal{E}(C_8H_9NO_2) =& \mid 0 \mid + \mid 0.55791 \mid + \mid -0.55791 \mid + \mid -2.0 \mid + \mid 2.0 \mid + \mid 4.0695 \mid + \mid -4.0695 \mid + \mid -5.3555 \mid + \mid 5.3555 \mid \\ & + \mid 6.2806 \mid + \mid -6.2806 \mid \end{aligned}$$

Maximum degree energy of paracetamol $MD\mathcal{E}(C_8H_9NO_2) = 36 \cdot 52702$. □

7. Randić Energy

It was in the year 1975, Milan Randić invented a molecular structure descriptor called Randić index which is defined as [22]

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

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 $R(G) := (r_{ij})$,

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

The characteristic equation of $R(G)$ is defined by $f_n(G, \rho) = det(\rho I - R(G)) = 0$. The roots of this equation 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 $\rho_1 \geqslant \rho_2 \geqslant \cdots \geqslant \rho_n$. 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 [5, 8, 10] and the references cited there in.

Theorem 7.1. *The Randić energy of paracetamol is,* $R\mathcal{E}(C_8H_9NO_2) = 6 \cdot 41212$

Proof. Randić matrix of paracetamol is,

$$R(C_8H_9NO_2) = \left(\begin{array}{c|ccccccccccc} & v_1 & v_2 & v_3 & v_4 & v_5 & v_6 & v_7 & v_8 & v_9 & v_{10} & v_{11} \\ \hline v_1 & 0 & \frac{1}{\sqrt{3}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ v_2 & \frac{1}{\sqrt{3}} & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{6}} \\ v_3 & 0 & \frac{1}{\sqrt{6}} & 0 & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ v_4 & 0 & 0 & \frac{1}{2} & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & 0 & 0 & 0 & 0 \\ v_5 & 0 & 0 & 0 & \frac{1}{\sqrt{6}} & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & 0 & \frac{1}{\sqrt{6}} & 0 \\ v_6 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{6}} & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & 0 & 0 \\ v_7 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{6}} & 0 & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & 0 & 0 \\ v_8 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{3}} & 0 & 0 & 0 & 0 \\ v_9 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{3}} & 0 & 0 & 0 & 0 \\ v_{10} & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \\ v_{11} & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \end{array}\right)$$

Characteristic equation is

$$432\rho^{11} - 1080\rho^9 + 939\rho^7 - 334\rho^5 + 22\rho^3 - \rho = 0$$

Randić eigenvalues are $\rho_1 = 0$, $\rho_2 \approx -0.16841$, $\rho_3 \approx 0.16841$, $\rho_4 \approx -0.5$, $\rho_5 \approx 0.5$, $\rho_6 \approx 0.62838$, $\rho_7 \approx -0.62838$, $\rho_8 \approx -0.90927$, $\rho_9 \approx 0.90927$, $\rho_{10} \approx 1.0$ and $\rho_{11} \approx -1.0$. Randić energy of paracetamol

$$\begin{aligned} R\mathcal{E}(C_8H_9NO_2) =& \mid 0 \mid + \mid -0.16841 \mid + \mid 0.16841 \mid + \mid 0.5 \mid + \mid -0.5 \mid + \mid 0.62838 \mid + \mid -0.62838 \mid + \mid -0.90927 \mid \\ &+ \mid 0.90927 \mid + \mid 1.0 \mid + \mid -1.0 \mid \end{aligned}$$

Randić energy of paracetamol is, $R\mathcal{E}(C_8H_9NO_2) = 6 \cdot 41212$. □

8. 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 $A_c(G) := (a_{ij})$, where

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

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 are the eigenvalues of $A_c(G)$. Since $A_c(G)$ is real and symmetric, its eigenvalues are real numbers and we label them in non-increasing order $\rho_1 \geqslant \rho_2 \geqslant \cdots \geqslant \rho_n$. 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 8.1. *The Color energy of paracetamol is,* $C\mathcal{E}(C_8H_9NO_2) = 20 \cdot 428$

Proof. Color matrix of paracetamol is,

$$A_c(C_8H_9NO_2) = \left(\begin{array}{c|cccccccccc} & v_1 & v_2 & v_3 & v_4 & v_5 & v_6 & v_7 & v_8 & v_9 & v_{10} & v_{11} \\ \hline v_1 & 0 & 1 & -1 & 0 & -1 & 0 & -1 & 0 & 0 & 0 & -1 \\ v_2 & 1 & 0 & 1 & -1 & 0 & -1 & 0 & -1 & -1 & -1 & 1 \\ v_3 & -1 & 1 & 0 & 1 & -1 & 0 & -1 & 0 & 0 & 0 & -1 \\ v_4 & 0 & -1 & 1 & 0 & 1 & -1 & 0 & -1 & -1 & -1 & 0 \\ v_5 & -1 & 0 & -1 & 1 & 0 & 1 & -1 & 0 & 0 & 1 & -1 \\ v_6 & 0 & -1 & 0 & -1 & 1 & 0 & 1 & -1 & -1 & -1 & 0 \\ v_7 & -1 & 0 & -1 & 0 & -1 & 1 & 0 & 1 & 1 & 0 & -1 \\ v_8 & 0 & -1 & 0 & -1 & 0 & -1 & 1 & 0 & -1 & -1 & 0 \\ v_9 & 0 & -1 & 0 & -1 & 0 & -1 & 1 & -1 & 0 & -1 & 1 \\ v_{10} & 0 & -1 & 0 & -1 & 1 & -1 & 0 & -1 & -1 & 0 & 1 \\ v_{11} & -1 & 1 & -1 & 0 & -1 & 0 & -1 & 0 & 0 & 1 & 0 \end{array}\right)$$

Characteristic equation is

$$\rho^{11} - 36\rho^9 + 88\rho^8 + 125\rho^7 - 636\rho^6 + 600\rho^5 + 118\rho^4 - 348\rho^3 + 40\rho^2 + 48\rho = 0$$

Color eigenvalues are $\rho_1 = 0$, $\rho_2 \approx -0.3433$, $\rho_3 \approx -0.5907$, $\rho_4 \approx 0.8257$, $\rho_5 \approx 1.0$, $\rho_6 \approx 1.2366$, $\rho_7 \approx 2.3795$, $\rho_8 \approx 2.0$, $\rho_9 \approx 2.7722$, $\rho_{10} \approx -2.6505$ and $\rho_{11} \approx -6.6295$. Color energy of paracetamol

$$\begin{aligned} C\mathcal{E}(C_8H_9NO_2) =& \mid 0 \mid + \mid -0.3433 \mid + \mid -0.5907 \mid + \mid 0.8257 \mid + \mid 1.0 \mid + \mid 1.2366 \mid + \mid 2.3795 \mid + \mid 2.0 \mid + \mid 2.7722 \mid \\ & + \mid -2.6505 \mid + \mid 6.4503 \mid \end{aligned}$$

Therefore $C\mathcal{E}(C_8H_9NO_2) = 20 \cdot 428$. □

9. Conclusion

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

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