Graph Energies of Anthraquinone: Energy, First Zagreb energy, Second Zagreb energy, Maximum Eccentricity Energy, Degree Product Energy, Degree Subtraction Energy

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Abstract:

In this paper I compute Energy, First Zagreb energy, Second Zagreb energy, Maximum Eccentricity Energy, Degree Product Energy, Degree Subtraction Energy of Anthraquinone.

Key words:

Anthraquinone, Eigen values, Energy, Characteristic equation, First Zagreb energy, Second Zagreb energy, Maximum Eccentricity Energy, Degree Product Energy, Degree Subtraction Energy.

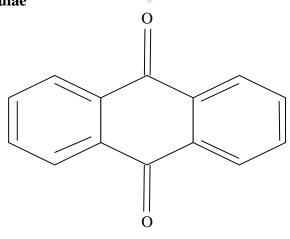
1. Introduction

Anthraquinones are active components of many plant blends which are used as medicines and exhibit laxative, diuretic, estrogenic and immunomodulatory effects. Anthraquinones are structurally related to anthracene and possess the 9,10-dioxoanthracene. Anthraquinones typically occur in their glycosidic forms. These compounds impart colour to plants and have been widely utilized as natural dyes. Anthraquinone is an important and widely used raw material for the manufacture of vat dyes, which are a class of water-insoluble dyes that can easily be reduced to a water soluble and usually colourless leuco form that readily impregnates fibres and textiles. In addition, they are also used as laxatives and possess antifungal and antiviral activities. It is also used as a seed dressing or in seed treatments. Other major uses are as a pesticide, as a bird repellent (especially for geese), and as an additive in chemical alkaline pulp processes in the paper and pulp industry.

So far, 79 naturally occurring anthraquinones have been identified which include emodin, physcion, cascarin, catenarin and Rhein. A large body of literature has demonstrated that the naturally occurring anthraquinones possess a broad spectrum of bioactivities, such as cathartic, anticancer, anti-inflammatory, antimicrobial, diuretic, Vaso relaxing and phytoestrogen activities, suggesting their possible clinical application in many diseases.

In this paper I compute Energy, Energy, First Zagreb energy, Second Zagreb energy, Maximum Eccentricity Energy, Degree Product Energy, Degree Subtraction Energy of Anthraquinone.

2. Structural and Molecular formulae

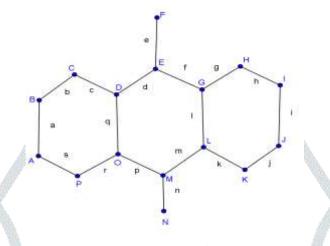


Molecular formulae: $C_{14}H_8O_2$

3. Energy of a Graph

The energy of a graph is one of the emerging concepts within graph theory. This concept serves as a frontier between chemistry and mathematics and is defined in1978 by I. Gutman [1] and originating from theoretical chemistry. In this paper we consider all graphs are simple without loops and multiple edges, finite and undirected. For standard terminology and notations related to graph theory, we follow Balakrishnan and Ranganathan [2]. The energy of a graph is zero if and only if it is trivial. The energy of a graph is one of the emerging concepts within graph theory. This concept serves as a frontier between chemistry and mathematics [3].

Let us consider the graph of Anthraquinone (i.e., Graph G) as shown in the following fig.



Graph G: Graph of Anthraquinone

Here the vertices A, B, C, D,, M, N, O, P are treated as the vertices $v_1, v_2, \dots, v_{13}, v_{14}, v_{15}, v_{16}$.

In general, G be a graph possessing n vertices and m edges. Let v_1, v_2, \dots, v_n be the vertices of G. Then the adjacency matrix A(G) of the graph G is the square matrix of order n whose (i, j) entry is defined as

$$a_{ij} = \begin{cases} 1 & \text{if } i \neq j \text{ and } v_i \text{ and } v_j \text{ are adjacent} \\ 0 & \text{if } i \neq j \text{ and } v_i \text{ and } v_j \text{ are not adjacent} \\ 0 & \text{if } i = j \end{cases}$$

The eigenvalues $\lambda_1, \lambda_2, \lambda_3, \dots, \lambda_n$ of the graph G are the eigen values of its adjacency matrix. Since A(G) is real symmetric, the eigen values of G are real numbers whose sum equal to zero.

The energy of a graph G is the sum of absolute values of the eigen values of a graph G and denoted it by E(G). Hence

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

E(G) will be referred as the ordinary energy of the graph G.

Energy of the Anthraquinone:

Adjacency matrix of Anthraquinone is shown in matrix 1.

The Characteristic equation is

 $x^{16} - 18x^{14} + 127x^{12} - 456x^{10} + 903x^8 - 998x^6 + 593x^4 - 168x^2 + 16 = 0$

The Eigen values of above characteristic equation are

 $\lambda_{1} = -2.49889, \lambda_{2} = 2.49889, \lambda_{3} = -2, \lambda_{4} = 2, \lambda_{5} = -1.6624, \lambda_{6} = 1.6624, \lambda_{7} = -1.49592, \lambda_{8} = 1.49592, \lambda_{9} = -1, \lambda_{10} = 1, \lambda_{11} = -1, \lambda_{12} = 1, \lambda_{13} = -0.757366, \lambda_{14} = 0.757366, \lambda_{15} = -0.424945, \lambda_{16} = 0.424945.$

The Energy of Anthraquinone is

$$\varepsilon(C_{14}H_8O_2) = |-2.49889| + |2.49889| + |-2| + |2| + |-1.6624| + |1.6624| + |-1.49592| + |1.49592| + |-1| + |1| + |-1|$$

 $+\left|l\right|+\left|-0.757366\right|+\left|0.757366\right|+\left|-0.424945\right|+\left|0.424945\right|$

= 21.679042

4. First Zagreb energy:

The first Zagreb matrix of a graph G is an $n \times n$ matrix denoted by $Z^{(1)}$ and whose elements are defined as

$$\left(Z^{(1)}\right)_{ij} = \begin{cases} d_i + d_j & \text{if } v_i v_j \in E(G) \\ 0 & \text{Otherwise} \end{cases}$$

The eigen values of $Z^{(1)}$ are denoted by $\lambda_1, \lambda_2, \lambda_3, \dots, \lambda_n$ and the first Zagreb energy [5] would be

$$ZE_1 = ZE_1(G) = \sum_{i=1}^n |\lambda_i|$$

First Zagreb energy of Anthraquinone:

The first Zagreb energy matrix of anthraquinone is as shown in matrix 2

The characteristic equation

$$x^{16} - 444x^{14} + 72502x^{12} - 5704604x^{10} + 234629745x^8 - 5118819904x^{10}$$

$$+56683460096x^4 - 274461114368x^2 + 377801998336 = 0$$

The eigen values are

$$\begin{split} \lambda_1 &= -13.7707 \,, \quad \lambda_2 &= -9.65924 \,, \quad \lambda_3 &= -8.45578 \,, \quad \lambda_4 &= -6.1601 \,, \quad \lambda_5 &= -4.6782 \,, \quad \lambda_6 &= -4.33745 \,\, \lambda_7 \,= -2.95472 \,, \\ \lambda_8 &= -1.47966 \,, \qquad \lambda_9 &= 1.47966 \,, \qquad \lambda_{10} \,= 2.95472 \,, \\ \lambda_{10} &= 2.95472 \,, \quad \lambda_{11} \,= 4.33745 \,, \\ \lambda_{12} &= 4.6782 \,, \quad \lambda_{13} \,= 6.1601 \,, \quad \lambda_{14} \,= 8.45578 \,, \\ \lambda_{15} &= 9.65924 \,, \\ \lambda_{16} &= 13.7707 \,. \end{split}$$

The first Zagreb energy =

|-13.7707| + |-9.65924| + |-8.45578| + |-6.1601| + |-4.6782| + |-4.33745| + |-2.95472| + |-1.47966| + |1.47966| + |2.95472| + |4.33745| + |4.6782| + |6.1601| + |8.45578| + |9.65924| + |13.7707| + |1.47966| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.47966| + |2.95472| + |1.4796| + |2.95472| + |2.95472| + |2.95472| + |2.95472| + |2.95472| + |2.95472| + |2.95472| + |2.95472| + |2.95472| + |2.95472| + |2.95472| + |2.95472| + |2.95472| + |2.95472| + |2.95472| + |2.95472| + |2.95472| + |2.95472| + |2.95472| + |2.95472| + |2.95472| + |2.95472| + |2.95472| + |2.95472| + |2.95472| + |2.95472| + |2.95472| + |2.95472| + |2.95472| + |2.95472| + |2.95472| + |2.95472| + |2.95472| + |2.9542| + |2.9542| + |2.9542| + |2.9542| + |2.9542| + |2.95

= 102.9917

5. Second Zagreb energy:

The second Zagreb matrix of a graph G is an $n \times n$ matrix denoted by $Z^{(2)}$ and whose elements are defined as

$$\left(Z^{(2)}\right)_{ij} = \begin{cases} d_i d_j & \text{if } v_i v_j \in E(G) \\ 0 & \text{Otherwise} \end{cases}$$

The eigen values of $Z^{(2)}$ are denoted by $\lambda_1, \lambda_2, \lambda_3, \dots, \lambda_n$ and the Second Zagreb energy [5] would be

$$ZE_2 = ZE_2(G) = \sum_{i=1}^n |\lambda_i|$$

Second Zagreb energy of Anthraquinone:

The Second Zagreb energy matrix of anthraquinone is as shown in the matrix 3.

The characteristic equation

 $x^{16} - 744x^{14} + 184706x^{12} - 20119020x^{10} + 1025265841x^8 - 25266388608x^6 + 1025265841x^8 - 25266588608x^6 + 10252665841x^8 - 25266588608x^6 + 1025266586x^6 + 1025266586x^6 + 1025266586x^6 + 1025266586x^6 + 102526658x^6 + 1025266586x^6 + 102526586x^6 + 102526586x^6 + 1025266586x^6 + 1025266586x^6 + 1025266586x^6 + 102526586x^6 + 1025266586x^6 + 102566586x^6 + 1025666x^6 + 1025666x^6 + 1025666x^6 + 102566x^6 + 102566x^6$

 $+284024641536x^4 - 1125692080128x^2 + 557256278016 = 0$

The eigen values are

 $\lambda_1 = -19.4735\,, \ \lambda_2 = -12.4215\,, \ \lambda_3 = -10.8502\,, \ \lambda_4 = -6.22152\,, \ \lambda_5 = -5.11306\,, \ \lambda_6 = -4.53458\,,$

$$\begin{split} \lambda_7 &= -2.6025 \,, \qquad \lambda_8 = -0.757644 \,, \qquad \lambda_9 = 0.757644 \,, \\ \lambda_{10} &= 2.6025 \,, \qquad \lambda_{11} = 4.53458 \,, \\ \lambda_{12} &= 5.11306 \,\, \lambda_{13} = 6.22152 \,, \\ \lambda_{14} &= 10.8502 \,, \\ \lambda_{15} &= 12.4215 \,, \\ \lambda_{16} &= 19.4735 \,. \end{split}$$

The second Zagreb energy =

 $\left|2.6025\right| + \left|4.53458\right| + \left|5.11306\right| + \left|5.11306\right| + \left|6.22152\right| + \left|10.8502\right| + \left|12.4215\right| + \left|19.4735\right| + \left|10.4735\right| + \left|10.4755\right| + \left$

= 123.949008

6. Maximum eccentricity energy of a graph:

The maximum eccentricity matrix is defined by

$$e_{ij} = \begin{cases} \max\left\{e\left(v_{i}\right), e\left(v_{j}\right)\right\} & \text{if } v_{i}v_{j} \in E(G)\\ 0 & \text{otherwise} \end{cases}$$

The characteristic polynomial of the maximum eccentricity matrix $M_e(G)$ is defined by

$$P(G,\lambda) = \det(\lambda I - M_e(G))$$

Where I is the unit matrix of order n. The maximum eccentricity eigenvalues of G are the eigen values of $M_e(G)$. Since $M_e(G)$ is real and symmetric with zero trace, then its eigenvalues are real numbers with sum is equal to zero.

The eigen values of $M_e(G) Z^{(2)}$ are denoted by $\lambda_1, \lambda_2, \lambda_3, \dots, \lambda_n$ and the maximum eccentricity energy [4] would be

$$EM_{e}(G) = \sum_{i=1}^{n} |\lambda_{i}|$$

Maximum eccentricity energy of Anthraquinone:

The Maximum eccentricity energy matrix of anthraquinone is as shown in the matrix 4.

The characteristic equation

$$x^{16} - 613x^{14} + 148842x^{12} - 18446842x^{10} + 1257760416x^8 - 47310175784x^6 + 930071976871x^4 - 8212346752925x^2 + 19335246997500 = 0$$

The eigen values are

$$\begin{split} \lambda_1 &= -14.0844 \,, \qquad \lambda_2 &= -12.8873 \,, \qquad \lambda_3 &= -9.35178 \,, \qquad \lambda_4 &= -9.02542 \,, \qquad \lambda_5 &= -6.66956 \,, \qquad \lambda_6 &= -5.78226 \,, \\ \lambda_7 &= -4.65573 \,, \lambda_8 &= -2.24496 \,, \qquad \lambda_9 &= 2.24496 \,, \\ \lambda_{10} &= 4.65573 \,, \qquad \lambda_{11} &= 5.78226 \,\, \lambda_{12} &= 6.66956 \,, \qquad \lambda_{13} &= 9.02542 \,, \\ \lambda_{14} &= 9.35178 \,, \\ \lambda_{15} &= 12.8873 \,, \\ \lambda_{16} &= 14.0844 \,. \end{split}$$

The Maximum eccentricity energy =

$$|-14.0844| + |-12.8873| + |-9.35178| + |-9.02542| + |-6.66956| + |-5.78226| + |-4.65573| + |-2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.24496| + |2.2449$$

= 129.40282

7. Degree Exponent Energy:

Let G be a simple graph with n vertices and m edges. Let v_1, v_2, \dots, v_n be the vertices of G. The degree d_i of a vertex v_i is the number of edges incident to v_i in G. The degree sum polynomial matrix is defined as $DE(G) = [de_{ij}]$, in which

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$$de_{ij} = \begin{cases} d_i^{d_j} & \text{if } i \neq j \\ 0 & \text{if } i = j \end{cases}$$

The characteristic polynomial $P_{DE(G)} = \det(\lambda I - DE(G))$ of a matrix DE(G) is called the degree exponent polynomial of G, where I is an identity matrix. The roots of the equation $P_{DE(G)} = 0$, denoted by $\lambda_1, \lambda_2, \lambda_3, \dots, \lambda_n$, are called the degree exponent eigen values of G and their collection is called the degree exponent spectrum of G. The sum of the absolute values of the degree exponent eigen values of G is called the degree exponent energy of G and is denoted by DEE(G). Thus

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

Degree Exponent Energy of Anthraquinone:

The Degree exponent energy matrix of anthraquinone is as shown in the matrix 5.

Characteristic Polynomial is

```
x^{16} - 14908x^{14} - 1367672x^{13} - 59048170x^{12} - 1478616272x^{11} - 22883018908x^{10} - 221699573528x^9 - 1298868562687x^8 - 3738235058080x^7 + 3994498377920x^6 + 82390524129792x^5 + 350048571618816x^4 + 803467935719424x^3 + 106988851814400x^2 + 76922634766336x + 228509902503936 = 0
```

The eigen values are

$$\begin{split} \lambda_1 &= -27.0338 \,, \qquad \lambda_2 &= -27.0331 \,, \qquad \lambda_3 &= -26.9938 \,, \qquad \lambda_4 &= -26.9807 \,, \qquad \lambda_5 &= -26.9456 \,, \qquad \lambda_6 &= -4.05875 \,, \\ \lambda_7 &= -4.03029 \,, \lambda_8 &= -4.02988 \,, \lambda_9 &= -3.99115 \,, \lambda_{10} &= -3.98599 \,, \qquad \lambda_{11} &= -3.96168 \,\, \lambda_{12} &= -3.95313 \,, \qquad \lambda_{13} &= -1.46835 \,, \\ \lambda_{14} &= -1 \,, \lambda_{15} &= 4.10226 \,, \lambda_{16} &= 161.366 \,. \end{split}$$

The degree exponent energy =

$$|-27.0338| |-27.0331| + |-26.9938| + |-26.9807| + |-26.9456| + |-4.05875| + |-4.03029| + |-4.02988| + |-3.99115| + |-3.98599| + |-3.96168| + |-3.95313| + |-1.46835| + |-1| + |4.10226| + |161.366|$$

= 330.93448

8. Degree product energy:

Let G be a graph with a vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$. The d_i be the degree of vertex v_i in G. The degree product matrix of a graph G is defined as $DP(G) = \lfloor dp_{ij} \rfloor$ in which

$$dp_{ij} = \begin{cases} (d_i)(d_j) & \text{if } i \neq j \\ 0 & \text{Otherwise} \end{cases}$$

The degree product energy of a graph G is defined as the sum of the absolute values of the eigen values of DP(G).

Degree Product energy of Anthraquinone:

The Degree Product energy matrix of anthraquinone is as shown in the matrix 6.

The characteristic polynomial is

 $x^{16} - 3564x^{14} - 176208x^{13} - 4459842x^{12} - 72550944x^{11} - 826741500x^{10} - 6885180432x^{9} - 6885180x^{9} - 6885180x^{9}$

 $-42830720919x^8 - 200847032576x^7 - 709523467200x^6 - 1869307407360x^5 - 186930740730x^5 - 186930740730x^5 - 186930740730x^5 - 186930740730x^5 - 186930740730x^5 - 186930740730x^5 - 186930740x^5 - 186930x^5 - 186930x^5$

- $-3595699413504x^{4} 4866174517248x^{3} 4347437432832x^{2}$
- -2275463135232x 522427760640 = 0

The eigen values are

$$\begin{split} \lambda_1 &= -9.07555 \,, \ \lambda_2 &= -9.03385 \,, \ \lambda_3 &= -9.01028 \,, \ \lambda_4 &= -8.96232 \,, \ \lambda_5 &= -8.95521 \,, \ \lambda_6 &= -5.95766 \,, \ \lambda_7 &= -4.1151 \,, \\ \lambda_8 &= -4.08312 \,, \ \lambda_9 &= -4.0706 \,, \ \lambda_{10} &= -3.97793 \,, \ \ \lambda_{11} &= -3.96722 \,\, \ \lambda_{12} &= -3.89755 \,, \ \ \lambda_{13} &= -3.88297 \,, \ \lambda_{14} &= -1.11796 \,, \\ \lambda_{15} &= -1 \,, \ \lambda_{16} &= 81.0756 \,. \end{split}$$

The degree product energy is

$$= |-9.07555| + |-9.03385| + |-9.01028| + |-8.96232| + |-8.95521| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-4.1151| + |-5.95766| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.956| + |-5.95$$

|-1.11796|+|-1|+|81.0756|=162.18292

9. Degree Subtraction energy:

Let G be a simple graph without loops and multiple edges on n vertices and m edges. Let $V(G) = \{v_i, v_j, \dots, v_n\}$ be the vertex set and E(G) be the edge set of G. The edge between the vertices u and v is denoted by uv. The degree of a vertex v_j in G is the number of edges incident to it and is denoted by $d_j = d_G(v_j)$. The degree subtraction matrix of a graph G is a square matrix of order n, defined as $DS(G) = [d_{ij}]$,

where

$$d_{ij} = \begin{cases} d\left(v_i\right) - d\left(v_j\right) & \text{if } i \neq j \\ 0 & \text{if } i = j \end{cases}$$

Then DS – polynomial of a graph G is the characteristic polynomial of degree subtraction matrix of G and is denoted by $\phi(G:\lambda)$. That is $\phi(G:\lambda) = \det(\lambda I_n - DS(G))$, where I_n is an identity matrix of order n. The roots of the equation $\phi(G:\lambda) = 0$ are called the DS – eigenvalues of G and they are labelled as $\lambda_1, \lambda_2, \lambda_3, \dots, \lambda_n$. The DS – energy [6] of a graph G, denoted by $E_{DS}(G)$ is defined as

$$E_{DS}\left(G\right) = \sum_{i=1}^{n} \left|\lambda_{i}\right|$$

Degree Subtraction energy of Anthraquinone:

The Degree Subtraction energy matrix of anthraquinone is as shown in the matrix 7.

The characteristic polynomial is

$$x^{16} + 112x^{14} = 0$$

The eigen values are
$$\lambda_1 = \lambda_2 = \lambda_3 = \lambda_4 = \lambda_5 = \lambda_6 = \lambda_7 = \lambda_8 = \lambda_9 = \lambda_{10} = \lambda_{11} = \lambda_{12} = \lambda_{13} = \lambda_{14} = 0$$

 $\lambda_{\scriptscriptstyle 15} = -10.583 i$, $\lambda_{\scriptscriptstyle 16} = 10.583 i$

The degree product energy is $E_{DS}(G) = \sum_{i=1}^{n} |\lambda_i| = 14.96662213$

[-	v_1	V_2	V ₃	v_4	V_5	V ₆	<i>V</i> ₇	V ₈	V ₉	<i>V</i> ₁₀	<i>v</i> ₁₁	<i>v</i> ₁₂	<i>v</i> ₁₃	<i>v</i> ₁₄	<i>V</i> ₁₅	<i>v</i> ₁₆
	<i>v</i> ₁	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1
	v_2	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
	V ₃	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0
	V_4	0	0	1	0	1	0	0	0	0	0	0	0	0	0	1	0
	<i>V</i> ₅	0	0	0	1	0	1	1	0	0	0	0	0	0	0	0	0
	V ₆	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
	V_7	0	0	0	0	1	0	0	1	0	0	0	1	0	0	0	0
$A(C_{14}H_8O_2) =$	V ₈	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0
	<i>V</i> ₉	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0
	<i>V</i> ₁₀	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0
	<i>v</i> ₁₁	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0
	<i>v</i> ₁₂	0	0	0	0	0	0	1	0	0	0	1	0	1	0	0	0
	<i>v</i> ₁₃	0	0	0	0	0	0	0	0	0	0	0	1	0	1	1	0
	<i>V</i> ₁₄	0	0	0	0	0	0	0	0	0	-0	0	0	1	0	0	0
	<i>v</i> ₁₅	0	0	0	1	0	0	0	0	0	0	0	0	1	0	0	1
	<i>V</i> ₁₆	1	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0

Matrix 1: Adjacency Matrix of Anthraquinone

		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}	v_{15}	v_{16}
1	<i>V</i> ₁	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	4
1	<i>v</i> ₂	4	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0
۱	<i>V</i> ₃	0	4	0	5	0	0	0	0	0	0	0	0	0	0	0	0
۱	<i>V</i> ₄	0	0	5	0	6	0	0	0	0	0	0	0	0	0	6	0
1	V ₅	0	0	0	6	0	4	6	0	0	0	0	0	0	0	0	0
۱	V ₆	0	0	0	0	4	0	0	0	0	0	0	0	0	0	0	0
1	V ₇	0	0	0	0	6	0	0	5	0	0	0	6	0	0	0	0
$ZE_1(G) = \iota $	<i>V</i> ₈	0	0	0	0	0	0	5	0	4	0	0	0	0	0	0	0
۱	V ₉	0	0	0	0	0	0	0	4	0	4	0	0	0	0	0	0
V	, 10	0	0	0	0	0	0	0	0	4	0	4	0	0	0	0	0
V	, 11	0	0	0	0	0	0	0	0	0	4	0	5	0	0	0	0
V	, 12	0	0	0	0	0	0	6	0	0	0	5	0	6	0	0	0
V	, 13	0	0	0	0	0	0	0	0	0	0	0	6	0	4	6	0
V	, 14	0	0	0	0	0	0	0	0	0	0	0	0	4	0	0	0
V	, 15	0	0	0	6	0	0	0	0	0	0	0	0	6	0	0	5
Lv	, 16	4	0	0	0	0	0	0	0	0	0	0	0	0	0	5	0

Matrix 2: First Zagreb Matrix of Anthraquinone

		v_1	v_2	<i>V</i> ₃	v_4	V_5	V_6	v_7	V ₈	V ₉	<i>V</i> ₁₀	<i>v</i> ₁₁	<i>v</i> ₁₂	<i>v</i> ₁₃	<i>v</i> ₁₄	<i>V</i> ₁₅	<i>v</i> ₁₆
	<i>v</i> ₁	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	4
	v ₂	4	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0
	V ₃	0	4	0	6	0	0	0	0	0	0	0	0	0	0	0	0
	V ₄	0	0	6	0	9	0	0	0	0	0	0	0	0	0	6	0
	<i>V</i> ₅	0	0	0	9	0	3	9	0	0	0	0	0	0	0	0	0
	V ₆	0	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0
	<i>v</i> ₇	0	0	0	0	9	0	0	6	0	0	0	9	0	0	0	0
$ZE_2(G) =$	v ₈	0	0	0	0	0	0	6	0	4	0	0	0	0	0	0	0
	<i>v</i> ₉	0	0	0	0	0	0	0	4	0	4	0	0	0	0	0	0
	<i>v</i> ₁₀	0	0	0	0	0	0	0	0	4	0	4	0	0	0	0	0
	<i>v</i> ₁₁	0	0	0	0	0	0	0	0	0	4	0	6	0	0	0	0
	<i>v</i> ₁₂	0	0	0	0	0	0	9	0	0	0	6	0	9	0	0	0
	<i>V</i> ₁₃	0	0	0	0	0	0	0	0	0	0	0	9	0	3	9	0
	<i>v</i> ₁₄	0	0	0	0	0		0	0	0	0	0	0	3	0	0	0
	<i>v</i> ₁₅	0	0	0	9	0	0	0	0	0	0	0	0	9	0	0	6
	_ <i>v</i> ₁₆	4	0	0	0	0	0	0	0	0	0	0	0	0	0	6	0

Matrix 3: Second Zagreb Matrix of Anthraquinone

	[v_1	v_2	V_3	v_4	V_5	V ₆	v_7	v_8	V ₉	<i>v</i> ₁₀	<i>v</i> ₁₁	<i>v</i> ₁₂	<i>v</i> ₁₃	<i>v</i> ₁₄	<i>v</i> ₁₅	v_{16}	
	v_1	0	7	0	0	0	0	0	0	0	0	0	0	0	0	0	7	
	v_2	7	0	7	0	0	0	0	0	0	0	0	0	0	0	0	0	
	v_3	0	7	0	6	0	0	0	0	0	0	0	0	0	0	0	0	
	v_4	0	0	6	0	5	0	0	0	0	0	0	0	0	0	5	0	
	v_5	0	0	0	5	0	5	5	0	0	0	0	0	0	0	0	0	
	v_6	0	0	0	0	5	0	0	0	0	0	0	0	0	0	0	0	
	<i>v</i> ₇	0	0	0	0	5	0	0	6	0	0	0	5	0	0	0	0	
$M_e(G) =$	v_8	0	0	0	0	0	0	6	0	7	0	0	0	0	0	0	0	
	v_9	0	0	0	0	0	0	0	7	0	7	0	0	0	0	0	0	
	<i>v</i> ₁₀	0	0	0	0	0	0	0	0	7	0	7	0	0	0	0	0	
	<i>v</i> ₁₁	0	0	0	0	0	0	0	0	0	7	0	6	0	0	0	0	
	<i>v</i> ₁₂	0	0	0	0	0	0	5	0	0	0	6	0	5	0	0	0	
	<i>v</i> ₁₃	0	0	0	0	0	0	0	0	0	0	0	5	0	5	5	0	
	<i>v</i> ₁₄	0	0	0	0	0	0	0	0	0	0	0	0	5	0	0	0	
	<i>v</i> ₁₅	0	0	0	5	0	0	0	0	0	0	0	0	5	0	0	6	
	v_{16}	7	0	0	0	0	0	0	0	0	0	0	0	0	0	6	0	
						J.				1	12							

Matrix 4: Maximum Eccentricity Matrix of Anthraquinone

	[v_1	v_2	<i>v</i> ₃	v_4	V_5	V_6	v_7	v_8	V ₉	<i>v</i> ₁₀	<i>v</i> ₁₁	<i>v</i> ₁₂	<i>v</i> ₁₃	<i>v</i> ₁₄	<i>v</i> ₁₅	v_{16}
	<i>v</i> ₁	0	4	4	8	8	2	8	4	4	4	4	8	8	2	8	4
	v_2	4	0	4	8	8	2	8	4	4	4	4	8	8	2	8	4
	v_3	4	4	0	8	8	2	8	4	4	4	4	8	8	2	8	4
	v_4	9	9	9	0	27	3	27	9	9	9	9	27	27	3	27	9
	v_5	9	9	9	27	0	3	27	9	9	9	9	27	27	3	27	9
	v_6	1	1	1	1	1	0	1	1	1	1	1	1	1	1	1	1
	<i>v</i> ₇	9	9	9	27	27	3	0	9	9	9	9	27	27	3	27	9
DE(G) =	v_8	4	4	4	8	8	2	8	0	4	4	4	8	8	2	8	4
	<i>v</i> ₉	4	4	4	8	8	2	8	4	0	4	4	8	8	2	8	4
	<i>v</i> ₁₀	4	4	4	8	8	2	8	4	-4	0	4	8	8	2	8	4
	<i>v</i> ₁₁	4	4	4	8	8	2	8	4	4	4	0	8	8	2	8	4
	<i>v</i> ₁₂	9	9	9	27	27	3	27	9	9	9	9	0	27	3	27	9
	<i>v</i> ₁₃	9	9	9	27	27	3	27	9	9	9	9	27	0	3	27	9
	<i>v</i> ₁₄	1	1	1	1	1	1	1	1	1	1	1	1	1	0	1	1
	<i>v</i> ₁₅	9	9	9	27	27	3	27	9	9	9	9	27	27	3	0	0
	<i>v</i> ₁₆	4	4	4	8	8	2	8	4	4	4	4	8	8	2	8	4
						-											

Matrix 5: Degree Exponent Matrix of Anthraquinone

		v_1	V_2	V ₃	v_4	V_5	V_6	v_7	V_8	V ₉	<i>V</i> ₁₀	<i>v</i> ₁₁	<i>v</i> ₁₂	<i>v</i> ₁₃	<i>v</i> ₁₄	<i>V</i> ₁₅	<i>v</i> ₁₆
	<i>v</i> ₁	0	4	4	6	6	2	6	4	4	4	4	б	б	2	6	4
	v_2	4	0	4	6	6	2	6	4	4	4	4	6	6	2	6	4
	<i>v</i> ₃	4	4	0	6	6	2	б	4	4	4	4	б	б	2	6	4
	<i>v</i> ₄	б	б	б	0	9	3	9	б	б	6	6	9	9	3	9	6
	<i>v</i> ₅	б	б	б	9	0	3	9	б	б	6	6	9	9	3	9	6
	v ₆	2	2	2	3	3	0	3	2	2	2	2	3	3	1	3	2
	<i>v</i> ₇	6	6	6	9	9	3	0	6	6	6	6	9	9	3	9	6
DP(G) =	<i>v</i> ₈	4	4	4	6	6	2	6	0	4	4	4	б	б	2	6	4
	v ₉	4	4	4	6	6	2	6	4	0	4	4	6	6	2	6	4
	V ₁₀	4	4	4	6	6	2	6	4	4	0	4	6	б	2	6	4
	<i>v</i> ₁₁	4	4	4	6	6	2	6	4	4	4	0	6	6	2	6	4
	<i>v</i> ₁₂	6	6	6	9	9	3	9	6	6	6	6	0	9	3	9	6
	<i>v</i> ₁₃	6	6	6	9	9	3	9	6	6	6	6	9	0	3	9	6
	<i>V</i> ₁₄	2	2	2	3	3	1	3	2	2	2	2	3	3	0	3	2
	<i>V</i> ₁₅	6	6	6	9	9	3	9	6	6	6	6	9	9	3	0	6
	V ₁₆	4	4	4	6	6	2	6	4	4	4	4	б	б	2	6	0
							-										

Matrix 6: Degree Product Matrix of Anthraquinone

		v_1	v_2	V ₃	v_4	V_5	V ₆	v_7	V ₈	V ₉	v_{10}	<i>v</i> ₁₁	<i>v</i> ₁₂	<i>v</i> ₁₃	<i>V</i> ₁₄	<i>V</i> ₁₅	v_{16}
	v ₁	0	0	0	-1	-1	1	-1	0	0	0	0	-1	-1	1	-1	0
	<i>v</i> ₂	0	0	0	-1	-1	1	-1	0	0	0	0	-1	-1	1	-1	0
	V ₃	0	0	0	-1	-1	1	-1	0	0	0	0	-1	-1	1	-1	0
	<i>v</i> ₄	1	1	1	0	0	2	0	1	1	1	1	0	0	2	0	1
	<i>V</i> ₅	1	1	1	0	0	2	0	1	1	1	1	0	0	2	0	1
	V ₆	-1	-1	-1	-2	-2	0	-2	-1	-1	-1	-1	-2	-2	0	-2	-1
	<i>v</i> ₇	1	1	1	0	0	2	0	1	1	1	1	0	0	2	0	1
DS(G) =	<i>v</i> ₈	0	0	0	-1	-1	1	-1	0	0	0	0	-1	-1	1	-1	0
	V ₉	0	0	0	-1	-1	1	-1	0	0	0	0	-1	-1	1	-1	0
	V ₁₀	0	0	0	-1	-1	1	-1	0	0	0	0	-1	-1	1	-1	0
	<i>v</i> ₁₁	0	0	0	-1	-1	1	-1	0	0	0	0	-1	-1	1	-1	0
	<i>v</i> ₁₂	1	1	1	0	0	2	0	1	1	1	1	0	0	2	0	1
	<i>V</i> ₁₃	1	1	1	0	0	2	0	1	1	1	1	0	0	2	0	1
	<i>V</i> ₁₄	-1	-1	-1	-2	-2	0	-2	-1	-1	-1	-1	-2	-2	0	-2	-1
	<i>v</i> ₁₅	1	1	1	0	0	2	0	1	1	1	- 1	0	0	2	0	1
	V ₁₆	0	0	0	-1	-1	1	-1	0	0	0	0	-1	-1	1	-1	0

Matrix 6: Degree Subtraction Energy Matrix of Anthraquinone

10. Conclusion:

In this article, I compute Energy, Energy, First Zagreb energy, Second Zagreb energy, Maximum Eccentricity Energy, Degree Product Energy, Degree Subtraction Energy of Anthraquinone.

References:

- 1. 1.I. Gutman. The energy of a graph, Ber. Math. Statist.S ekt. forschungsz. Graz 103(1978) 1-22
- 2. R. Balakrishnan, The energy of a graph, Lin. Algebra Appl.387(2004) 287-295.
- 3. I. Gutman, Chemical graph theory- The mathematical connection, in : J.R.Sabin, E.J.Brandas(Eds.), Advances in Quantum chemistry 51, Elsevier, Amsterdam, 2006, pp.125-138.
- 4. Ahmed M. Naji and N.D. Soner, The Maximum Eccentricity Energy of a Graph, International Journal of Scientific & Engineering Reasearch, Vol 7,Issue 5,May 2016.
- 5. Nader Jafari Rad, Akbar Jahanbani, Ivan Gutman, Zagreb Energy and Zagreb Estrada Index of Graphs, Communications in Mathematical and in Computer chemistry,79 (2018) 371-386
- 6. H. S. Ramane, K. C. Nandeesh, G. A. Gudodagi, B.Zhou, Degree substraction eigen values and energy of graphs, Computer Science Journal of Moldova, Vol 26, no.2(77), 2018