COMPUTATIONAL ANALYSIS OF ENERGY OF SOME OF THE GRAPHS USING MATGRAPH

Muhammad Javed Ayub

Scholar, University of Lahore

Corresponding Author: *
Muhammad Javed Ayub

Abstract

The story begins with an awkward problem whose solution could not be categorized into any known branch of mathematics of the day. Slowly, in the 19th century, more mathematical curiosities began to be lumped into the same category of graphs. By the 20th century, graph theory had become a rigorous field with countless applications in not only mathematics itself but also many scientific disciplines. Graph theory is a mathematical study of graphs. Leonard Euler was the first person to solve a problem scientifically through graphs in 1736. It is the study of graphs through nodes and edges. The birth of graph theory is often considered to have taken place in 1736 when the Swiss mathematician solved a problem of the seven bridges of Konigsberg. Today, graph theory has become one of the most interesting and innovative fields of mathematics. Graph theory is a growing field and is being applied to areas of physics, computer science, pattern studies, and communication networks. Graph theory has a great contribution to the field of chemistry. The energy of a graph is the sum of the absolute values of the eigenvalues of the adjacency matrix of the graph. It is the study of the spectral properties of a graph by studying the characteristic polynomial and eigenvectors of matrices associated with the graph, such as its adjacency matrix. In this study, we will find the energy of the octagonal quadrilateral network with n-quadrilaterals and n-octagons.

INTRODUCTION

1.1 History of Graph

The Seven Bridges of Konigsberg[1], a famous 1736 paper by the eminent Swiss mathematician Leonhard Euler, is regarded as the foundational work on graph theory. He solved this problem with the help of the first graph, which is considered to be the foundational stone of this vast field of mathematics. The city of Konigsberg is now in Russia. In addition to this the concept of graph theory is a link between chemistry and mathematics.It was first proposed by Ivan Gutman in 1978, but its chemical roots date back to the 1940s. A large number of mathematicians from all over the world started working on it. The term 'Graph energy' gained popularity when a paper was published in 1978, describing it by taking the adjacency matrix, calculating its eigenvalues, and by summing the absolute values of the eigenvalues[2]. This was the first time the term was used. In a symposium in Stift Rein, Austria it was discussed.Gutman did a lot of work on graph theory and showed that this energy of graph is a structural descriptor for π electrons system[3] that is satu- rated.He defined the ordinary energy of the graph K and represented by $E = E(K)$ and drew it link to the overall electron energy of a class of organic molecule. It was the link between the characteristic polynomial of G and E(G) as well as the lower and upper constraints on E's vertices and edges.

1.2 Chemical Graph Theory

Chemical graph theory is a subfield of chemistry . It deals with chemical graphs. In molec- ular graph vertex are atoms and edges are the bonds between the two molecules. This concept ignores the hydrogen atoms in the molecule. Topological indices have also been used in chemical graph theory [4].

1.3 Spectra of Graph

The spectral analysis of graph theory [5] studies the relation between graph attributes and the spectrum of adjacency matrix or Laplace matrix. By studying the spectrum of the far away stars in distinct galaxies the astronomers figure out how far away those stars are. The temperature, atmosphere and environment is also studied. Eigenvalues are connected to all invariants. They also create links between two different aspects of the graphs. The study of eigenvalues has increased over the years and has become important in graph theory.

1.4 Energy of Graph

Graph theory deals with the vertices and edges. It is linked with the molecule so that the atoms are considered as vertices and the chemical bond is represented by edges. we ignore the hydrogen atoms in the molecular structure. Gutman introduced a molecular descriptor to estimate the molecule's total π-electrons energy [3]. If a graph has n vertices and n edges then set representing the vertices V = $\{m_1, m_2, m_3, m_4, \dots m_n\}$ and set of edges E=\{y1,y2,y3,y4, ...yn\}

$$a_{ij} = \begin{cases} 1, if\ V_i = V_j \\ 0, otherwise \end{cases}$$

If $\lambda_1 > \lambda_2 > \lambda_3 > \lambda_4 \dots > \lambda_n$ are the eigenvalues of the given graph A(k). The greatest value λ_1 is called the graph's spectral radius. Then by taking the sum of absolute values of the eigenvalues of a given adjacency matrix of a graph, K is termed the energy of the graph [6] denoted by

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

1.5 Estrade Index of Graph

Ernesto Estrada introduced the term Estrada Index[7] for the first time in year 2000 while working on protein molecules. Since then several reports were communicated on the basis of this index in the field of chemical and non chemical graphs. This index is widely used in several fields, such as chemistry, thermodynamics. If λ_1 , λ_2 , λ_3 , $\lambda_4 \dots \lambda_n$, are the eigenvalues of the graph G, then the Estrada index is defined as

$$EE(G) = \sum_{n=1}^{n} e^{\lambda_i}$$

The distance Estrada Index was recently studied in which the distance matrix eigenvalues were employed and not the adjacency matrix. The set of all eigenvalues is known as the spectrum of the graph G[12]. of graph theory. A topological index [8] is a molecular descriptor that specifies a property of a molecular structure. The most important is to determine the chemical properties and their generalization.

1.6 Topological Index of Graph

Topological indices are the most essential aspect

1.7 Eigen Values

Eigenvalues are not only important in

mathematics but also in different branches of economics, chemistry and other fields of science. Eigenvalues are used to predict certain properties of a molecule in chemistry. That's is why chemistry and mathematics are related to one another. Antibonding level is connected with positive eigenvalues, and bonding level is linked with negative eigenvalues. Whereas the non-bonding level is linked with zero eigenvalues. [9]

$$A = \begin{bmatrix} 2 & 3 & 4 & 5 \\ 1 & 2 & 3 & 4 \\ 6 & 7 & 8 & 9 \\ 4 & 5 & 6 & 7 \end{bmatrix}$$

If a matrix has equal number of rows and columns, then it is a square matrix.

Rectangular Matrix
If the rows and columns are not equal, then it is called a rectangular matrix. Example
$$A = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 6 & 7 & 7 & 9 \\ 4 & 3 & 6 & 2 \end{bmatrix}$$

If the matrix remains unchanged when we interchange its rows and columns then such matrix is termed as symmetric matrix and the process is called transposing a matrix. example
$$A = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 2 & 7 & 7 & 9 \\ 3 & 7 & 6 & 6 \\ 4 & 9 & 6 & 2 \end{bmatrix}$$

This matrix is called symmetric matrix as it remains the same when we interchange its rows and columns. A symmetric matrix is always a square matrix. The following terms and definitions are used in this research.

Adjacency Matrix
A square matrix which is formed with assigning the value one when the two vertex are adjacent to one another and zero when they are not adjacent to one another. The adjacency matrix is always symmetric.

Simple Graph
In this thesis simple graphs are used. The simple graphs are one which have no loop and no multiple edges between them.

Graph
A graph is a nonempty set U of vertices and set V

of edges which may or may not be empty. Some interesting work have been done.and some of them have been listed below

Four color problem
One of the importent concept in graph theory is the four color problem(Thomas, 1998) which states that "is it true that any map drawn in the plane may have its regions colored with four colors, so that any two regions having a same border have different colors." Similarly, other important work done by mathematicians in different fields are listed below.
- **Shortest path problem**
- **Pabble motion problem**
- **Art gallery problem**
- **Three cottage problem**
- **Solving sudoku' s problem.**

Chapter 2 Literature Review
Literature Review
2.1 Matrices
A collection of numbers in rows and columns is called a matrix. The horizontal arrangement is a row, and the vertical is a column. If a matrix has U rows and V columns, then the matrix order is UxV. For example

2.2 **Basic concepts of graph theory**

Graph

A graph is considered to be a nonempty set U of vertices and set V of edges which may or may not be empty.

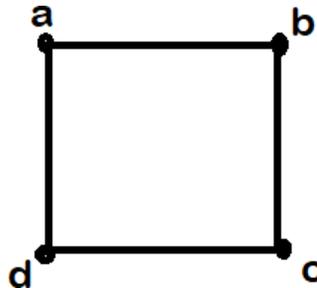**Example :**

Figure 1:Graph

In the graph, the vertex set P = {p,q,r,s} Q ={ab , bc , cd , da}

Edge

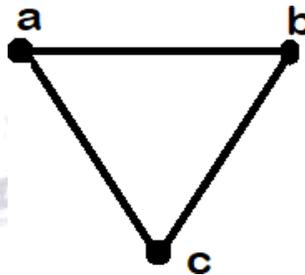For the any two vertices the line joining between them is termed as an edge.

Figure 2: Edge

Example

In the figure, the lines joining the vertices ab, bc, and ca are called edges.

Loop

A graph is a nonempty set U of vertices and set V of edges which may or may not be empty.

Example

Figure 3: loop

Degree of Vertex

Number of edges that are adjacent to any given vertex.

Example: In the figure the degree of vertex a, b, c, d each is 2 while the degree of vertex e is 0.
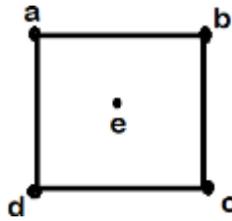
Figure 4: Degree of Vertex

Order of the Graph

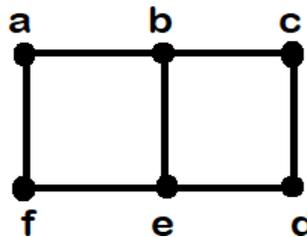The order of the graph can be determined out by counting the number of vertices of the given graph.

Figure 5: Order of the Graph

Example: In this graph, the order of the graph is 6

Size of the Graph

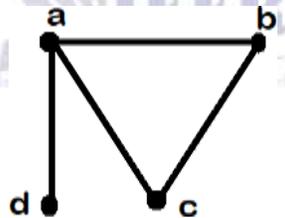The number of edges in a graph is termed as the size of graph.

Figure 6: Size of the Graph

Example: In the figure the size of the graph is 4.

Adjacent vertices

If two of the vertices are joined by a common edge, they are termed as adjacent vertices.

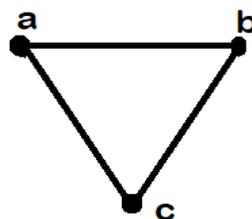**Example:** In the graph all vertices are adjacent vertices.

Figure 7: Adjacent vertex

Adjacent edges

If two edges are linked together by a common vertex between them, they are called adja- cent edges. Here in this graph the adjacent edges are d and e.

Example:

Figure 8: adjacent edges

2.3 Types of graphs

Null Graph

If all the vertices of a given graph are not connected by any of the edge with other vertices then the graph is termed as null graph.
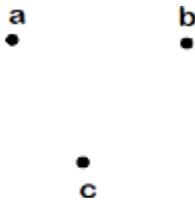
Example

Figure 9: Null Graph

Trivial Graph

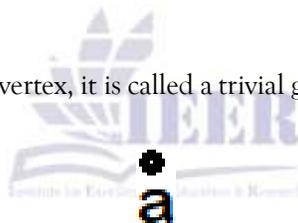If a graph has no edges and only a single vertex, it is called a trivial graph.

Example

Figure 10 : Trivial Graph

Simple Graph

A simple graph is the one which has no parallel edges and no loops.
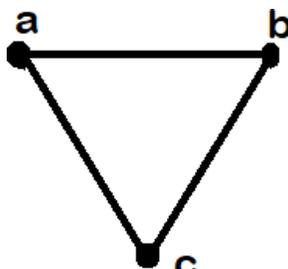
Example:

Figure 11: Simple Graph

Connected Graph

A graph is called connected only if a path can be found between each pair of unique ver- tices in a network.
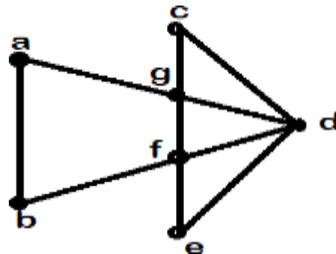
Example:

Figure 12: Connected Graph

Disconnected Graph

A graph is said to be disconnected only if it is not connected.
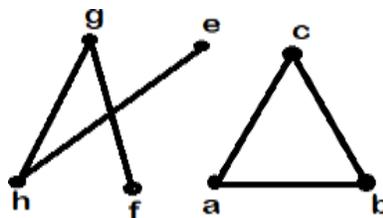
Example

Figure 13 : Disconnected Graph

Regular Graph

If each node of a graph has the same degree, it is termed a regular graph.
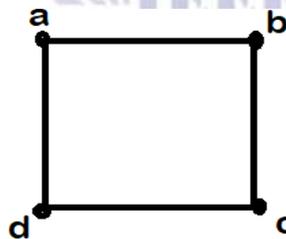
Example:

Figure 14: Regular Graph

Complete Graph

If every node is adjacent to all other nodes in the graph, then the graph is said to be a complete graph. It is denoted by K.
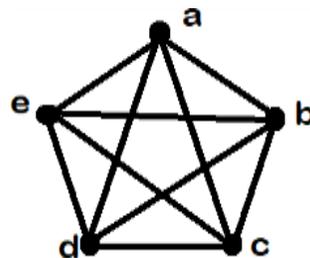
Example

Figure 15 : Complete Graph

Cycle Graph

A cycle geaph is a simple graph with 'p' vertices where (p≥ 3) and 'p' edges is termed as cycle graph if all the

edges of the graph form a complete cycle of length 'p'. If the degree of every vertex of the graph is 2, then it is termed a cycle graph.

Example
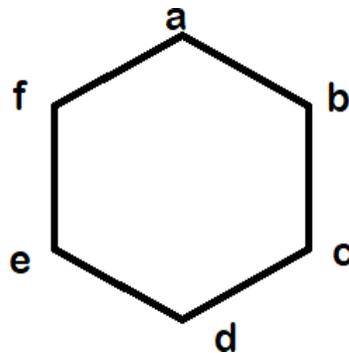
Figure 16: Cycle

Wheel Graph

A wheel graph with 'n' vertices may be constructed from a cycle graph C by introducing a fresh vertex that is adjacent to every other vertex.
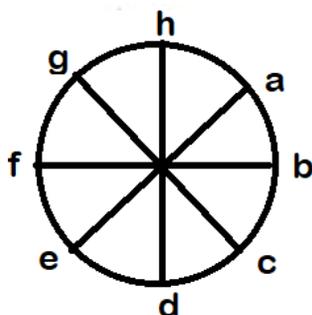
Example:

Figure 17: Wheel

Bipartite Graph

A collection of vertices of a graph that has been divided into two separate sets in such a way that no two vertices from the same set are joined to one another is known as bipertite graph.
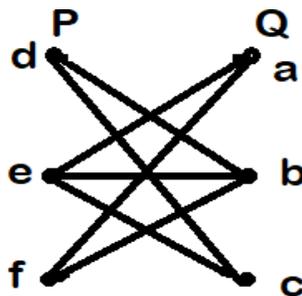
Example

Figure 18: Bipartite Graph

Complete Bipartite Graph

In a bipartite graph, if every vertex in the first set P is linked with every other vertex in the second set Q, then it is termed a complete bipartite graph.

Example
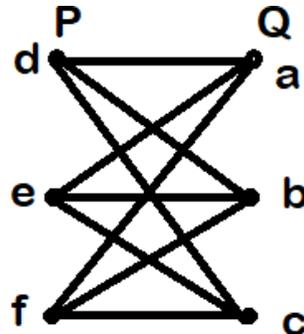
Figure19: Complete Bipartite Graph

Tree

If we take a connected graph in such a way that we don't find any cycle in it, then the graph is termed as Tree.

Example:

Figure 20: Tree

Planer Graph

A graph in which any two randomly selected edges do not intersect each other is called a planer graph.

Example:

Figure 21: Planner Graph

Forest

A disconnected collection of trees is called a Forest.

Example:

Figure 22: Forest

2.4   Matrices Associated with Graphs

3.3 Matrices in Graph Theory We are all familiar with the definition of matrix and the basics and principals of matrix operations. There ar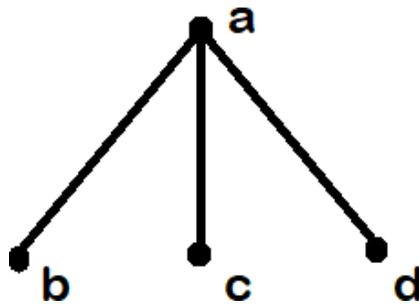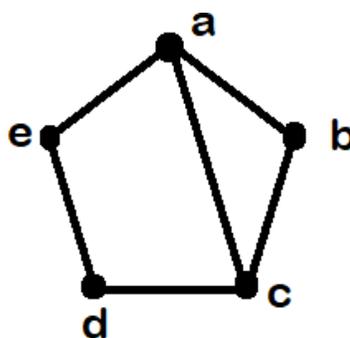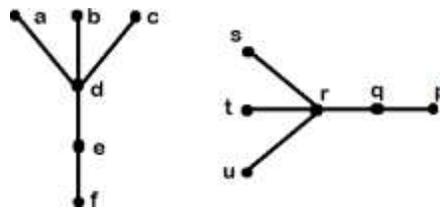e certain matrix concepts that are associated with the graph theory and this research work have been explained. The matrix A with order s x t having s rows and t columns is represented as

$$A = \begin{bmatrix} k_{11} & k_{12} & k_{13....} & k_{1t} \\ k_{21} & k_{22} & k_{23....} & k_{2t} \\ k_{31} & k_{32} & k_{33....} & k_{3t} \\ ...\ddots & ...\ddots & ...\ddots & ...\ddots \\ k_{s1} & k_{s2} & k_{s3} & k_{st} \end{bmatrix}$$

And eigenvalues corresponding to its characteristic equation $|A - \lambda I| = 0$ are exact roots. The eigen values are real if matrix A is symmetric.

Spectrum matrix

Spectrum matrix [10] is a collection of different eigenvalues. Let it be $\lambda_1, \lambda_2, \lambda_3, \lambda_4 \quad \lambda_n$, of every n-dimensional matrix with their multiplicities $m_1, m_2, m_3, m_4, ... m_t$, respectively such that $m_1 + m_2 + m_3 + m_4 ...... + m_t = n$ is denoted by

Example:

$$A = \begin{bmatrix} t_{11} & t_{12} & t_{13....} & t_{1n} \\ t_{21} & t_{22} & t_{23....} & t_{2n} \\ k_{31} & k_{32} & k_{33....} & k_{3t} \\ ...\ddots & ...\ddots & ...\ddots & ...\ddots \\ k_{s1} & k_{s2} & k_{s3} & k_{st} \end{bmatrix} \begin{bmatrix} e_1 \\ e_2 \\ e_3 \\ e_4 \\ ... \\ e_n \end{bmatrix}$$

Adjacency Matrix

The adjacency matrix of a graph represented by A(G) = $[k_{ij}]$ an n- dimensional real square symmetric matrix whose $[k_{ij}]$ th entry is explained as For undirected graph adjacency matrix is symmetric.
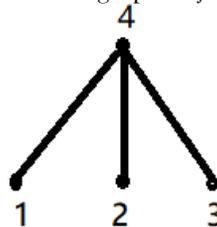

Figure 23: Undirected Graph

$$A = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix}$$

Incidence Matrix

The n x m matrix C = $[c_{ij}]$ that creates incidence matrix [11] of G has n rows that represent the n vertices and m columns that represent the m edges.
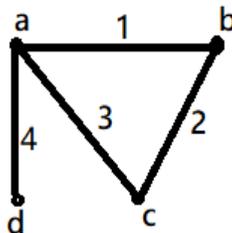
Example:

Figure 24: Incidence Matrix Graph

$$A = \begin{bmatrix} 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix}$$

Degree Matrix

Degree matrix represented by the symbol D = D(G) is determined by D(G)=[M_{ij}], where It is obvious that the degree matrix of G is the diagonal matrix whose leading diagonal elements are the degree of the vertices of G.

Its eigenvalues are with a result d_i = $deg[v_i]$, where i = 1, 2, 3,......,n.

2.5   Some Old Results on Graph Energy

In addition to determining the upper limit for the energy of a strongly quotient graph in terms of the adjacency matrix, Adiga and R.K. Zaferani also discovered two eigenvalues of a highly quotient graph [12]. An improved upper limit, two new lower bounds and better lower and higher bounds for the Estrada index of highly quotient graphs involving graph energy and several other graph invariants were discovered by B. Bozkurt, C. Adiga, and D. Bozkurt. As well as a Nordhaas-Gaddum-type solution for the highest eigenvalue, K.C. Das discovered the lower and upper limits for the reciprocal distance (Harary) matrix of a connected (molecular) graph's eigenvalue [13]. B.Zhou and co-workers investigated the Laplacian energy L(G) of simple graphs and its relationship to the Graph energy E(G) [14]. Bo Zhou and I. Gutman developed many new Laplacian energies and developed Laplacian energy characteristics [15]. Singaraj K. Ayyaswamy developed and studied the Signless Laplacian Estrada index, as well as the lower and upper limits for simple graphs in terms of vertices and edges. Bao-Xuan Zhu discovered extremal graphs with a certain connectivity k that maximize the Laplacian Estrada index.

The highest Laplacian Estrada index for n-vertex graphs with a given matching number was also determined by the author. N. Trinajstic, D. Janezic, A. Milicevic, S. Nikolic, and D. Janezic Graph Theoretical Matrices in Chemistry presents a range of graph matrices that are often encountered in chemical graph theory. This book covers adjacency matrices, incidence matrices, distance matrices and graphical matrices. The majority of the presented graph theoretical matrices are used as sources of molecular descriptors known as topological indices, which

have a wide variety of applications in QSPR (quantitative structure property relationship) and QSAR (quantitative structure activity relationship) [16]. In Seidel switching and graph energy, W. H. Haemers discusses the Seidel switching of graphs and defines the Seidel energy. In certain rare cases, Seidel switching does not change the spectrum and hence the energy. There is an infinite family of situations with extremely high energy where Seidel switching changes the spectrum but not the energy, and he has established a bottom limit hypothesis that 2(n1) is the smallest value of S(G) over all graphs with n vertices. Certain Results on the Laplacian Energy of a Graph by LIU Ying and WU Baofeng analyzes the link between the Laplacian energy and the singular values of the Laplacian matrix and derives certain restrictions. Energy changes caused by eliminating edges and vertices from a graph are also explored. Yang, Yi-Qiu, Xu, and Hu, Chang-Yu extended adjacency matrix indices and their ap- pli- cations introduces new topological indices based on the extended adjacency matrices of the molecules investigated.

The findings show that the indices have a high discriminatory power and are substantially linked with a wide range of organic compound physicochemical properties and biological activities [17]. According to Meenakshi's and Havana, all of the energies, including Laplacian, distance, and Harary, are the same. The maximum degree energy is much superior to any of the other energies that have been presented. Maximum degree energy dominates the other energies among the stated energies [18]. Graphs of order are studied by Jafari, Jahan Bani, and Gutman First Zagreb matrix is the square matrix whose V_i $_j$-element is equal to the sum of the degrees of neighboring vertices V_i and V_j, or zero otherwise.

The energy of the graph is a vast field. In different fields and situations different energies are calculated which represent different aspects of the molecule. The following are few energies which are widely used in graph theory.

2.6 Maximum Degree Energy

We can simply define the maximum degree energy of a simple connected graph K [18] as the sum of the absolute values of eigenvalues of the maximum degree matrix of a graph k.
Where

$$M_{ij} = \begin{cases} \max(d_i, d_j), & if\, v_i, v_j \varepsilon\, E(K), \\ 0 & otherwise, \end{cases}$$

Minimum Degree Energy

The minimum degree energy[19] of a simple connected graph K can be calculated by taking sum of the absolute values of eigenvalues of the minimum degree matrix of a graph K. Here, where

$$M_{ij} = \begin{cases} \min(d_i, d_j), & if\, v_i, v_j \varepsilon\, E(K), \\ 0 & otherwise, \end{cases}$$

2.7 Randić Energy

The randic´ energy of a simple connected graph K in [20] is the sum of the absolute values of eigenvalues of the randic´ matrix. where

$$r_{ij} = \begin{cases} \dfrac{1}{\sqrt{d_i d_j}}, & if\, v_i, v_j \varepsilon\, E(K), \\ 0 & otherwise, \end{cases}$$

2.8 Seidel Energy

Seidel energy[21] of a graph K is another kind of energy which can be calculated by taking the sum of the

absolute values of eigenvalues of the seidel matrix of K. where

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

2.9 Sum-Connectivity Energy

The sum-connectivity energy[22] of a graph K is another kind of energy that can be calculated by taking the sum of the absolute values of the eigenvalues of the sum-connectivity matrix. Here, where

$$r_{ij} = \begin{cases} \dfrac{1}{\sqrt{d_i d_j}}, & if\, v_i, v_j \varepsilon\, E(G), \\ 0 & otherwise, \end{cases}$$

2.10 Applications of Graph Theory

Applications of graph theory in different fields of such as computer science, engineering, social sciences, physics, and chemistry. Graph theory is used in a variety of network creations and their analysis for optimization. This helps in finding their anomalies and i to increase their performance. It also helps to optimize any problem. One of the famous problems is the salesman problem. This helps to optimize logistical problems to reduce cost and increase efficiency. It also helps to create cryptographic algorithms. For example RSA cryptosystem. In the field of computer science, it is used to model data structures such as trees. With the help of graph theory, problems of shortest path and minimum spanning tree have been solved. In the field of Biology complex metabolic and protein interaction networks are studied. This helps to identify drug targets. In social sciences, graph theory is used to study social networks such as Facebook and Twitter. This helps people to have suitable friend suggestions and potential customers. Graph theory also helps in the field of physics to study quantum field theory and spin systems. This helps to predict their properties. Graph theory has also helped to solve many problems, such as the four color problem, Three cottage problem, and many more.

Methodology
Software Used in Research

Different software has been used in my research to find the adjacency matrix, eigenvalues, and to make the images of the chain of molecules. Finding the adjacency matrix of a large molecule is not an easy task. The same is the case in finding the eigenvalues. Following soft- wares have been used.

3.1 Matlab

MATLAB is one of the most powerful tools that can be used to draw the graph, import data from other software in the form of matrices, and find their eigenvalues. It is also used to find the energy of the graph. MATLAB [23] has several toolboxes that can be used in most other explorations, which are really helpful when using graph theory for a large-scale real-time project.

3.2 CamDraw

Drawing the graph of chemical compounds according to their formulae is one of the tasks that chemists come across during their professional life. It is really difficult to draw the graph with hands as such graphs are not perfect, and it is not advisable to present them before others or in publications. ChemDraw is one such tool that makes life easier for professionals in this field.

3.3 Topocluj

It is a software used to find the adjacency matrix of a large size complex graph. It helps to find the adjacency matrix of those graphs whose matrix cannot be found manually.

3.4   Matgraph

Matagraph [24] is a toolbox for working with simple graphs in MATLAB. The goal is to make interactive graph theory exploration simple and efficient.

Chapter 4: Results

4.1   Tetracene($C_{18}H_{12}$)

A polycyclic aromatic hydrocarbon, Tetracene[25] is an organic compound that consists of four linearly fused benzene rings, which form a type called "Linear acene." It has various chemical and scientific applications. Its Chemical formula is $C_{18}H_{12}$, and its Molar Mass is 228.29 grams per mole. It appears to be a yellow crystalline powder.
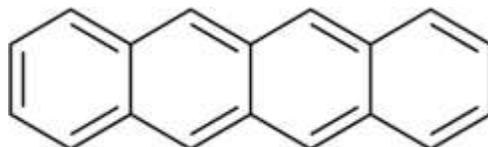

Figure 25: Tetracene

It does not have a positive or negative charge in its structure making it a non polar compound.its melting point is 398 degree centigrade. It is insoluble in water but soluble in toulene and chloroform.It5 is a excellent conductor of electric charge so it is widely used in organic field-effect transistor (OFETs) and organic light emitting diodes(OLEDs).It has property of converting heat energy to electrical energy so it is used in solar cells.It is quiet sensitive to air and light so protective measures are taken to prevent its degradation.

Table 1: linear equations for the energy of Tetracene($C_{18}H_{12}$)

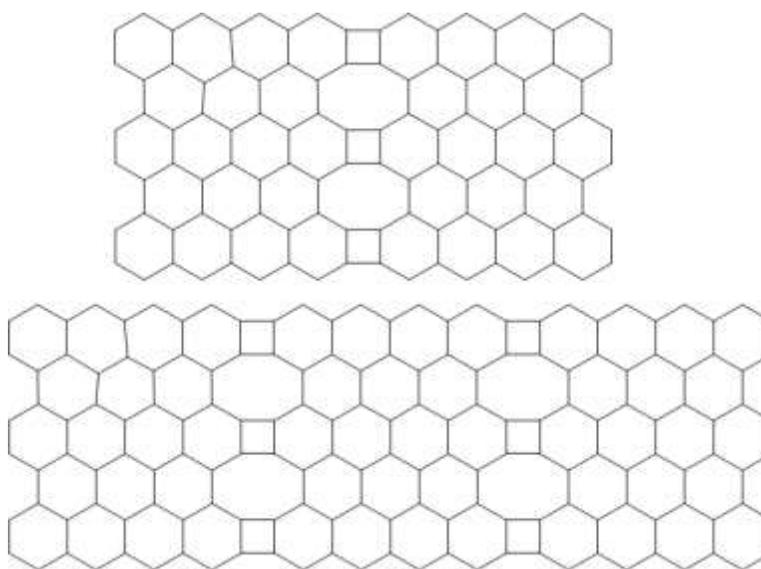| Quadratic equations for the energy of Tetracene($C_{18}H_{12}$)	
(m ,n)	Energy($C_{18}H_{12}$)
(1,n)	$-0.0006n^2 + 25.592n - 0.6608$
(2,n)	$0.0069n^2 + 53.186n - 1.2666$
(3,n)	$-0.0837n^2 + 81.359n - 2.2016$

Figure 25: Tetracene Chain

Table 2: Quadratic equation obtained from the 'curves' coefficients

Quadratic equation obtained from the 'curves' coefficients as shown in table 1	
(n)	Energy($C_{18}H_{12}$)
n^2	$-0.049m^2 + 0.1547m - 0.1062$
n	$0.258m^{l}2 + 26.883m - 1.612$
1	$0.1624m^2 - 1.747m + 1.5778$

Table 3: Actual and Predicted values of energy of ($C_{18}H_{12}$) showing negligible error. This proves that the equations formed can be used to find energy of any size of molecule.

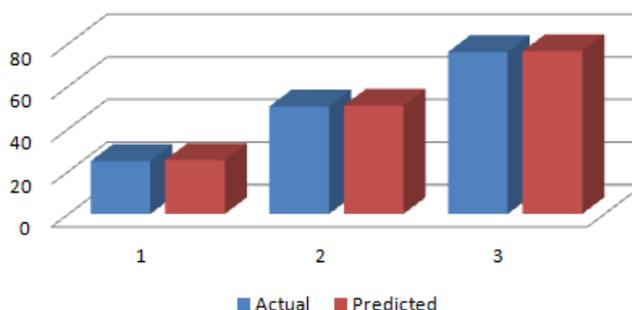| Actual and Predicted values of energy of ($C_{18}H_{12}$)			
(m ,n)	E_{actual}	$E_{Perdicted}$	Error
(1 , n)	24.9308	25.3593	0.4285
(2 ,n)	50.5212	50.8868	0.3656
(3 , n)	76.1104	76.4133	0.3029

Figure 27: Actual vs predicted energy of Tetracene

The above graph shows the comparison between the actual values calculated and the values based on the equations generated on our predictions and assumptions. As we move further towards more complex molecule structure, we see that the two values move side by side.

4.2   Octagonal Quadrilateral Graph
The Octagonal Quadrilateral graph is as shown in figure. It is in the shape of a regular octagon with a square shape attached to one edge of it.
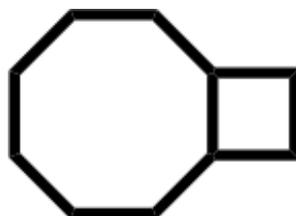

Figure 28: Octagonal Quadrilateral

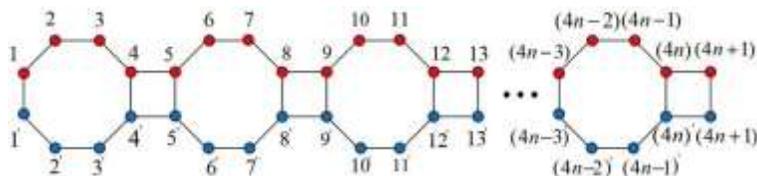The long chain of Octagonal Quadrilateral graph is as shown in figure.

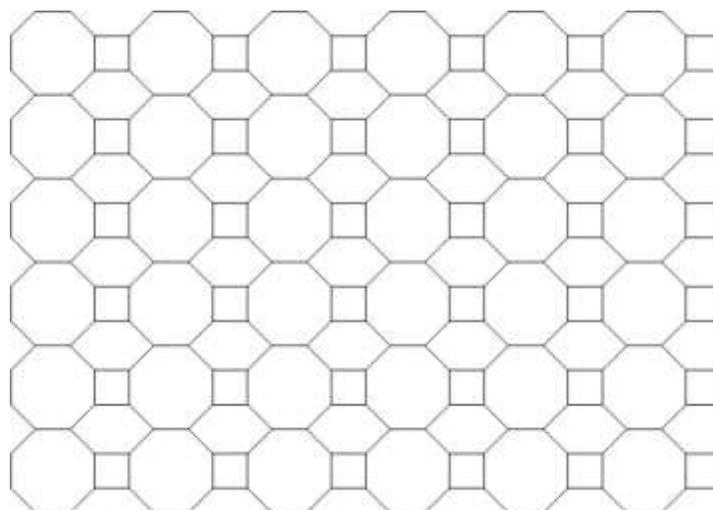**Figure 29: Octagonal Quadrilateral Graph**

Figure30: Octagonal-Quadrilateral Graph

Table 4: Quadratic equation for the energy of Octagonal Quadrilateral Graph

Quadratic equation for the energy of Octagonal Quadilateral Graph	
(m ,n)	Energy
(1 , n)	$4\times10^{-05}n^2 + 10.926n + 1.816$
(2 ,n)	$8\times10^{-0.5}n^2 + 19.891n + 3.3269$
(3 , n)	$6\times10^{-5}n^2 + 28.808n + 5.1308$
(4 , n)	$4\times10^{-05}n^2 + 37.737n + 6.723$
(5 , n)	$6\times10^{-05}n^2 + 46.636n + 8.456$
(6 , n)	$4\times10^{-05}n^2 + 55.543n + 10.093$
(7 , n)	$5\times10^{-05}n^2 + 64.482n + 11.761$
(8 , n)	$4\times10^{-05}n^2 + 73.403n + 13.429$
(9, n)	$4\times10^{-05}n^2 + 82.325n + 15.096$
(10 , n)	$4\times10^{-05}n^2 + 91.246n + 16.764$

The above graph shows the comparison between the actual values calculated and the values based on the equations generated on our predictions and assumptions. As we move further towards more complex molecule structure, we see that the two values move side by side showing negligible error. This proves that the equations formed can be used to find energy of any size of molecule.

Table 5: Quadratic equation obtained from the 'curves' coefficients

Quadratic equation obtained from the 'curves' coefficients as shown in table 1	
(n)	Energy
n^2	$-2 \times 10^{-07} m^2 - 2 \times 10^{-07} m + 6 \times 10^{-05}$
n	$0.0036 m^2 + 8.8912 m + 2.0759$
1	$0.0004 m^2 + 1.6627 m + 0.0975$

Table 6: Actual and Predicted values of energy of the octagonal Quadrilateral graph

Actual and Predicted values of energy of octagonal Quadrilateral graph			
(m ,n)	E_{actual}	$E_{Perdicted}$	Error
(6 , 1)	67.412	65.641	1.771
(6 ,2)	122.715	121.194	1.5213
(6 , 3)	178.025	176.74666	1.2783
(6 , 4)	233.174	232.2997	0.8743
(6 , 5)	288.326	287.853	0.473
(6 , 6)	343.403	343.406	0.003
(6 , 7)	398.703	398.9595	0.2565
(6 , 8)	453.910	454.513	0.603
(6 , 9)	509.099	510.0665	0.9675
(6 , 10)	564.297	565.620	1.323

The above graph shows the comparison between the actual values calculated and the values based on the equations generated on our predictions and assumptions. As we move further towards more complex molecule structure, we see that the two values move side by side showing negligible error. This proves that the equations formed can be used to find energy of any size of molecule.
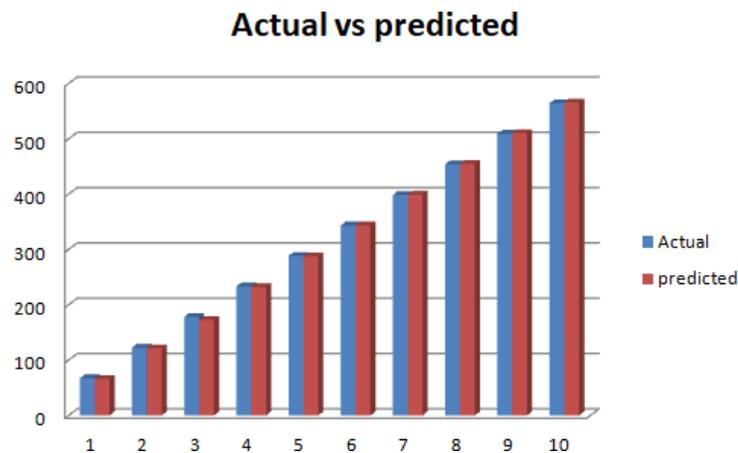
Figure 31: Actual vs predicted energy of the graph

Table 7: Quadratic equations for the Estrada Index of Octagonal Quadrilateral

Quadratic equations for the Estarada Index of Octagonal Quadrilateral	
(m ,n)	Estrada Index
(1,n)	$0.0001n^2 + 22.625n + 2.5568$
(2,n)	$0.00005n^2 + 0.42.703n + 5.0642$
(3,n)	$-0.0002n^2 + 62.781n + 7.5716$
(4,n)	$-0.00002n^2 + 82.858n + 10.079$
(5,n)	$0.0036n^2 + 102.9n + 12.641$
(6,n)	$-0.00002n^2 + 123.01n + 15.098$

Table 8: Actual and Predicted values of Estrada Index of octagonal Quadrilateral graph

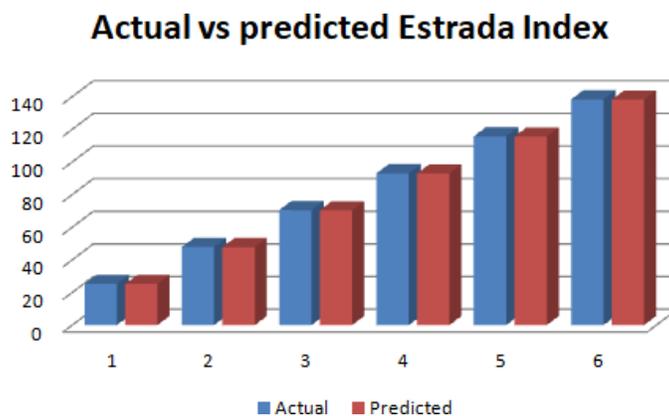| Actual and Predicted values of Estrada Index of octagonal Quadrilateral graph			
(m ,n)	E_{actual}	$E_{Perdicted}$	Error
(1 , 1)	25.1822	25.1797	0.0025
(1 ,2)	47.8085	47.7703	0.0382
(1 ,3)	70.4345	70.3608	0.0737
(1 , 4)	93.0610	92.9517	0.1093
(1 , 5)	115.687	115.543	0.144
(1 , 6)	138.3149	138.1347	0.1802

Figure 32: Actual vs predicted values of estrada Index of the graph

Chapter 5: Conclusions

Conclusions

As we have seen from the above results, the general equations formed during the research process when compared with the actual values of energy of the graph, the difference or the error that is seen during the comparison process is negligible. This shows that the work done, the assumptions made, and the process applied on these graphs correctly reflect the true results. Hence, we can conclude that the energy of the graph with the long chain can also be calculated using these equations. As we have worked on Tetracene, we have successfully formed the energy equations that reflect the true values. same is the case with Estrada Index. The values of the Estrada Index calculated using the generalized equations successfully match with the actual values calculated.

References

Wang, S. (2004). Graph theory. Beijing: Press of Beijing Institute of Technology.

Gutman, I., Li, X., Zhang, J. (2009). Graph energy. Analysis of Complex Networks: From Biology to Linguistics, 145-174.

Gutman, I., Furtula, B. (2017). The Total [pi] - Electron Chemica Acta, 90(3), 359-369.

Trinajstic, N. (2018). Chemical graph theory. Routledge.

Energy Saga. Croatica

Chung, F. R. (1997). Spectral graph theory (Vol. 92). American Mathematical Soc.

Gutman, I., Li, X., Zhang, J. (2009). Graph energy. Analysis of Complex Networks: From Biology to Linguistics, 145-174.

Gutman, I., Deng, H., Radenkovic, S. (2011). The Estrada index: an updated survey.

Selected Topics on Applications of Graph Spectra, Math. Inst., Beograd, 155-174.

Hansen, P. J., Jurs, P. C. (1988). Chemical applications of graph theory. Part I. Fundamentals and topological indices. Journal of Chemical Education, 65(7), 574.

Spielman, D. (2012). Spectral graph theory. Combinatorial scientific computing, 18, 18.

Spielman, D. (2012). Spectral graph theory. Combinatorial scientific computing, 18,18.

Van Nuffelen, C. (1976). On the incidence matrix of a graph. IEEE Transactions on Circuits and Systems, 23(9), 572-572.

Klee, W. E. (2004). Crystallographic nets and their quotient graphs. Crystal Research and Technology: Journal of Experimental and Industrial Crystallography, 39(11), 959-968.

Gutman, I., Li, X., Zhang, J. (2009). Graph energy. Analysis of Complex Networks:

From Biology to Linguistics, 145-174.

Mohar, B., Alavi, Y. , Chartrand, G. , Oellermann , O. R. (1991). The Laplacian spectrum of graphs. Graph theory, combinatorics, and applications, 2(871-898), 12.

Spielman, D. (2012). Spectral graph theory. Combinatorial scientific computing, 18,

Costa, P. C., Evangelista, J. S., Leal, I., Miranda, P. C. (2020). Chemical graph theory for property modeling in QSAR and QSPR—charming QSAR QSPR. Mathematics, 9(1), 60.

Gupta, S., Yamuna, M. (2018). Physiochemical Properties of Medicines-Using Graph Eccentricity and Multiple Regression. Research Journal of Pharmacy and Technology, 11(9), 4112-4118.

Adiga, C., Smitha, M. (2009). On maximum degree energy of a graph. Int. J. Contemp. Math. Sci, 4(8), 385-396.

Gutman, I., Li, X., Zhang, J. (2009). Graph energy. Analysis of Complex Networks: From Biology to Linguistics, 145-174.

Gutman, I., Furtula, B., Bozkurt, S˛ . B. (2014). On randic´ energy. Linear Algebra and its Applications, 442, 50-57.

Nageswari, P., Sarasija, P. B. (2014). Seidel energy and its bounds. Int. J. Math. Anal, 8(57), 2869-2871.

Gutman, I. , Furtula, B. (2 0 1 9). Graph energies and their applications. Bulletin (Academfie s´erbe des scfiences et des arts. Cflasse des scfiences mathe´matfiques et naturelles. Sciences math´ematiques), (44), 29-45.

Scheinerman, E. R. (2008). Matgraph: a MATLAB toolbox for graph theory.

Department of applied mathematics and statistics, the Johns Hopkins University, Baltimore, Maryland, 1-7.

Scheinerman, E. R. (2008). Matgraph: a MATLAB toolbox for graph theory.

Department of applied mathematics and statistics, the Johns Hopkins University, Baltimore, Maryland, 1-7.

Raji, M., Jayalalitha, G. (2021). Eccentric Distance Sum in Chemical Compounds Graph Using Domination. In Proceedings of First International Conference on Mathematical Modeling and Computational Science: ICMMCS 2020 (pp. 23-33). Springer Singapore.