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THE ENERGY OF GRAPH: A NEW PERSPECTIVE

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ABSTRACT

The ordinary energy of graph is defined as the sum of the absolute values of Eigen values obtained from the adjacency matrix of the molecular graph for a given chemical compound. There has always been a limitation that the adjacency matrix obtained from the molecular graph has no information about the bonds and the atoms connected. Hence to overcome this limitation, we are considering the atom connectivity and connectivity matrix which gives more information about the types of bonds and atom connectivity of a chemical compound in the molecular graph and the matrix calculations. In this paper we define atom connectivity energy and connectivity energy also find energy of few hydrocarbons and their comparison with the ordinary energy.

Keywords: Adjacency matrix, Energy of Graph, Domination Matrix, Distance Domination Matrix Atom Connectivity Matrix, Connectivity Matrix, Molecular Graph, Laplacian Matrix

1. INTRODUCTION

The concept of graph energy arose in theoretical chemistry where certain numerical quantities, as the heat of formation of a hydrocarbon are related to total π electron energy that can be calculated as the energy of corresponding molecular graph. The molecular graph is representation of molecular structure of a hydrocarbon whose vertices are the position of carbon atoms and two vertices are adjacent, if there is a bond connecting them.
Eigenvalues and eigenvectors provide insight into the geometry of the associated linear transformation. The energy of a graph is the sum of the absolute values of the eigenvalues of its adjacency matrix. From the pioneering work of Coulson (Zhou, 2017) there exists a continuous interest towards the general mathematical properties of the total π electron energy $\mathcal{E}$ as calculated within the framework of the Huckel Molecular Orbital (HMO) model. These efforts enabled one to get an insight into the dependence of $\mathcal{E}$ on molecular structure. The properties of $\varepsilon(G)$ are discussed in detail in (Basak et al. ,1988) (Zhou, 2007) (Coulson, 1940) (Bonchev et al., 2002).

The energy so obtained represents the physical and chemical properties of the molecules. The above concept energy of graph has few limitations. In energy of graph various types of bonds are represented in the form a single edge, more over different atoms are also represented as nodes and the corresponding adjacency matrix too have neither information of the various types of atoms nor the types of the bonds in the molecule hence the significant of double bond, triple bond or atoms cannot be interpreted in energy of graph. Hence, we are overcoming the above limitations by introducing the various energy of graph through atom connectivity matrix (ACM) and in general connectivity matrix (CM) (Cvetkovic, 1980) (Gutman et al., 2017).

The purpose of this study is to investigate the various energy of graph through the new perspective of atom connectivity matrix and in general connectivity matrix. The current study is innovative as the connectivity matrix approach has not yet been studied. Moreover, the new study will explore the various possible applications in the field of applied sciences.

2. LITERATURE REVIEW

Over the last 30 years there has been extensive research on these topics with hundreds of research papers published in recent years all over the Globe. It is noteworthy that there are more than 60 different types of energy of graph defined with various applications in the field of sciences particularly in chemistry (Gutman, 1978).

In order to display the structure of the molecule on a computer screen there must be a specific input about the information about the molecule. Till date there is no uniform accepted specific way to input the information about the molecules in the computer. Connectivity matrix and atom connectivity matrix are one among many ways to represent the atom in the computer which have the information of bonds and the atoms connectivity (Cvetkovic, 1980) (Gutman et al, 2017).

Various researchers introduced many different types of energy of graphs and produced various results in the energy of graph which led to the significant interest among mathematicians all over the world. The lists of few familiar energies of graph are given as below (Gutman, 1978). Energy of Graph, Domination Energy of Graph, Distance Energy of Graph, Distance Domination Energy of Graph, Laplace Energy of Graph, Distance Laplace Energy of Graph, Signless Laplace Energy of Graph, Signless Distance Laplace Energy of Graph, Sum-Connectivity Energy, Color Energy, and others. To show the molecule on the computer screen, the computer must be told about molecular structure. Molecular modeling software requires that this information be provided in the form of a sketch on the screen which is usually done with a mouse or some other pointing device, or prompts the user for a name of the disk file where the information is stored.

Most of the energies of graph defined above are oriented towards adjacency matrix. Atom connectivity and connectivity matrix was introduced by S.C. BASAK and V.R. MAGNUSON in 1988 (Cvetkovic, 1980). For computer representation of molecules, Spialter (Sampath, 2010; Gutman et al., 2017) introduced the concept of atom connectivity matrix. Mathavi Manisekar and S. Lalitha have also obtained few results in Dissociation Energy for Amino Acids (Gutman, 1986).

The atom-connectivity matrix, denoted by ACM, has been proposed by Spialter (1963, 1964, 1964) for the use in computer-oriented chemical nomenclature. This matrix represents the structural formula of a molecule and is given by

$$[ACM]_{ij} = \begin{cases} b_{ij} & \text{if vertices } i \text{ and } j \text{ are adjacent} \\ s_i & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

where b_{ij} is the bond order between atoms i and j, and s_i stands for the chemical symbol of the atom i, for matrix calculation s_i is considered to be zero. The values of bond orders in most cases are 1, 1.5, 2, and 3 for single, aromatic, double and triple bonds, respectively.

If only the molecular skeleton without hydrogen atoms is considered, then one gets the hydrogen-suppressed structure. Spialter called the corresponding structural matrix the hydrogen-suppressed atom-connectivity matrix, denoted by HS-ACM (Spialte, 1964, 1964; Von Knop et al., 1975). The advantage of using HS-ACM instead of ACM at that time (1964) was in reducing the size of the matrix to save computer time.

Similarly in the atom connectivity matrix the diagonal includes the atomic number of the connected atom then the matrix is called connectivity matrix denoted by CM**,** similarly hydrogen-suppressed connectivity matrix is denoted by HS-CM.

$$[CM]_{ij} = \begin{cases} b_{ij} & \text{if vertices } i \text{ and } j \text{ are adjacent} \\ n_i & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

where b_{ij} is the bond order between atoms i and j, and n_i stands for the atomic number of the atom i.

3. RESEARCH METHODOLOGY

3.1 Definition and Notation (Frank, 1975; Gutman, 2017; Gutman, 1978)

Graph Energies

All the equations has been chosen so as to be fully analogous to the definition of Energy of Graph:

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

where $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq, \ldots\ldots\ldots, \geq \lambda_n$ are the ordinary graph eigenvalues, that is, the eigenvalues of the adjacency matrix of G $A(G)$

Distance Energy of Graph,

$$E_D = E_D(G) = \sum_{i=1}^{n} |\mu_i|$$

where $\mu_1 \geq \mu_2 \geq \mu_3 \geq, \ldots\ldots\ldots, \geq \mu_n$ are the eigenvalues obtained from distance matrix of G $D(G)$

Laplace Energy of Graph,

$$E_L = E_L(G) = \sum_{i=1}^{n} |\psi_i|$$

where $\psi_1 \geq \psi_2 \geq \psi_3 \geq, \ldots\ldots\ldots, \geq \psi_n$ are the eigenvalues obtained from Laplacian matrix $L(G)$ of G, $L(G) = d(G) - A(G)$, $A(G)$ and $d(G)$ are the adjacency matrix and diagonal matrix with vertex degree of *G*

Signless Laplace Energy of Graph,

$$E_{SL} = E_{SL}(G) = \sum_{i=1}^{n} |q_i|$$

where $q_1 \geq q_2 \geq q_3 \geq, \ldots\ldots\ldots, \geq q_n$ are the eigenvalues obtained from Signless Laplacian matrix $SL(G)$of G, $SL(G) = d(G) + A(G)$, $A(G)$ and $d(G)$ are the adjacency matrix and diagonal matrix with vertex degree of *G*

Laplace distance energy

$$E_{LD} = E_{LD}(G) = \sum_{i=1}^{n} |\beta_i|$$

where $\beta_1 \geq \beta_2 \geq \beta_3 \geq, \ldots\ldots\ldots, \geq \beta_n$ are the eigenvalues obtained from Laplacian distance matrix $LD(G)$ of G, $LD(G) = d(G) - D(G)$, $D(G)$ and $d(G)$ are the distance matrix and diagonal matrix with vertex degree of *G*

Signless Laplace distance energy,

$$E_{SLD} = E_{SLD}(G) = \sum_{i=1}^{n} |\rho_i|$$

where $\rho_1 \geq \rho_2 \geq \rho_3 \geq, \ldots\ldots\ldots, \geq \rho_n$ are the eigenvalues obtained from Laplacian distance matrix $LD(G)$ of G, $LD(G) = d(G) + D(G)$, $D(G)$ and $d(G)$ are the distance matrix and diagonal matrix with vertex degree of *G*.

Domination energies

Domination Energy of Graph: where $\kappa_1 \geq \kappa_2 \geq \kappa_3 \geq,\ldots\ldots\ldots,\geq \kappa_n$ are the eigenvalues obtained from the domination matrix of G $A_\gamma(G)$

Distance Domination Energy of Graph, $E_{D\gamma} = E_{D\gamma}(G) = \sum_{i=1}^{n} |\sigma_i|$

where $\sigma_1 \geq \sigma_2 \geq \sigma_3 \geq,\ldots\ldots\ldots,\geq \sigma_n$ are the eigenvalues obtained from distance domination matrix of G $D_\gamma(G)$

Laplace Domination Energy of Graph, $E_{L\gamma} = E_{L\gamma}(G) = \sum_{i=1}^{n} |\alpha_i|$

where $\alpha_1 \geq \alpha_2 \geq \alpha_3 \geq,\ldots\ldots\ldots,\geq \alpha_n$ are the eigenvalues obtained from Laplacian Domination matrix $L_\gamma(G)$ of G, $L_\lambda(G) = d(G) - A_\gamma(G)$, $A_\gamma(G)$ and $d(G)$ are the domination matrix and diagonal matrix with vertex degree of *G*

Signless Laplace Domination Energy of Graph, $E_{SL\gamma} = E_{SL\gamma}(G) = \sum_{i=1}^{n} |\delta_i|$

where $\delta_1 \geq \delta_2 \geq \delta_3 \geq,\ldots\ldots\ldots,\geq \delta_n$ are the eigenvalues obtained from Signless Laplacian domination matrix $SL(G)$of G, $SL_\gamma(G) = d(G) + A_\gamma(G)$, $A_\gamma(G)$ and $d(G)$ are the adjacency matrix and diagonal matrix with vertex degree of *G*

Laplace distance domination energy: $E_{LD\gamma} = E_{LD\gamma}(G) = \sum_{i=1}^{n} |\phi_i|$

where $\phi_1 \geq \varphi_2 \geq \varphi_3 \geq,\ldots\ldots\ldots,\geq \phi_n$ are the eigenvalues obtained from Laplacian distance domination matrix $LD_\gamma(G)$ of G, $LD\gamma(G) = d(G) - D_\gamma(G)$, $D_\gamma(G)$ and $d(G)$ are the distance domination matrix and diagonal matrix with vertex degree of *G*

Signless Laplace distance domination energy: $E_{SLD\gamma} = E_{SLD\gamma}(G) = \sum_{i=1}^{n} |\eta_i|$

where $\eta_1 \geq \eta_2 \geq \eta_3 \geq,\ldots\ldots\ldots,\geq \eta_n$ are the eigenvalues obtained from signless Laplacian distance domination matrix $SLD_\gamma(G)$ of G, $SLD\gamma(G) = d(G) + D_\gamma(G)$, $D_\gamma(G)$and $d(G)$ are the distance domination matrix and diagonal matrix with vertex degree of *G*

Laplacian energies

From the above Laplace and signless Laplace energies, one could obtain the Laplacian and Signless Laplacian energies by subtracting $\frac{2m}{n}$ from the respective Eigen values, where m is the number of edges and n is the number of vertices of a graph G. Here the Laplacian energy $\hat{E}$ (number of edges with bound) and E (number of edges without bound) are separately evaluated.

$$E_{Ln} = E_{Ln}(G) = \sum_{i=1}^{n} \left| \psi_i - \frac{2m}{n} \right|$$

$$E_{SLn} = E_{SLn}(G) = \sum_{i=1}^{n} \left| q_i - \frac{2m}{n} \right|$$

$$E_{LnD} = E_{LnD}(G) = \sum_{i=1}^{n} \left| \beta_i - \frac{2m}{n} \right|$$

$$E_{SLnD} = E_{SLnD}(G) = \sum_{i=1}^{n} \left| \rho_i - \frac{2m}{n} \right|$$

$$E_{Ln\gamma} = E_{Ln\gamma}(G) = \sum_{i=1}^{n} \left| \alpha_i - \frac{2m}{n} \right|$$

$$E_{SLn\gamma} = E_{SLn\gamma}(G) = \sum_{i=1}^{n} \left| \delta_i - \frac{2m}{n} \right|$$

$$E_{LnD\gamma} = E_{LnD\gamma}(G) = \sum_{i=1}^{n} \left| \phi_i - \frac{2m}{n} \right|$$

$$E_{SLnD\gamma} = E_{SLnD\gamma}(G) = \sum_{i=1}^{n} \left| \eta_i - \frac{2m}{n} \right|$$

Atom connectivity energy and Connectivity energy

The energy calculates with respect to the atom connectivity matrix and connectivity matrix is called atom connectivity energy and connectivity energy respectively. Illustrations are given below:

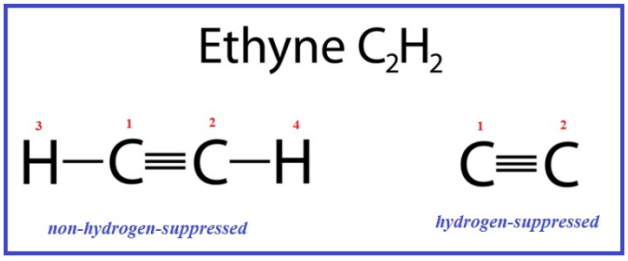

Figure 1: Ethyne

Table 1: Initial Matrices

non-hydrogen-suppressed matrix

Adjacency Matrix

	1	2	3	4
1	0	1	1	0
2	1	0	0	1
3	1	0	0	0
4	0	1	0	0

Atom Connectivity Matrix

	1	2	3	4
1	0	3	1	0
2	3	0	0	1
3	1	0	0	0
4	0	1	0	0

Connectivity Matrix

	1	2	3	4
1	6	3	1	0
2	3	6	0	1
3	1	0	1	0
4	0	1	0	1

hydrogen-suppressed matrix

	1	2
1	0	1
2	1	0

	1	2
1	0	3
2	3	0

	1	2
1	6	3
2	3	6

Domination matrix is obtained from the adjacency matrix $A(G)$ of G by replacing the a_{ii} element by 1 if and only if $v_i \in S$. S being the dominating set. For connectivity matrix $a_{ii} = n_i + 1$, n_i stands for the atomic number of the atom i and 1 if and only if $v_i \in S$. S being the dominating set.

Table 2: Domination Matrices

non-hydrogen-suppressed matrix

Domination Matrix

	1	2	3	4
1	1	1	1	0
2	1	1	0	1
3	1	0	0	0
4	0	1	0	0

Domination Atom Connectivity Matrix

	1	2	3	4
1	1	3	1	0
2	3	1	0	1
3	1	0	0	0
4	0	1	0	0

Domination Connectivity Matrix

	1	2	3	4
1	7	3	1	0
2	3	7	0	1
3	1	0	1	0
4	0	1	0	1

hydrogen-suppressed matrix

	1	2
1	1	1
2	1	0

	1	2
1	1	3
2	3	0

	1	2
1	7	3
2	3	6

Distance matrix $D(G)=[d_{ij}]$, where d_{ij} is the shortest distance between the vertex v_i and v_j in *G*. For connectivity matrix $a_{ij}=d_{ij}+b_{ij}$, b_{ij} is the bond order between atoms i *and* j .

Table 3: Distance Matrices

non-hydrogen-suppressed matrix

Distance Matrix

	1	2	3	4
1	0	1	1	2
2	1	0	2	1
3	1	2	0	3
4	2	1	3	0

Distance Atom Connectivity Matrix

	1	2	3	4
1	0	4	2	2
2	4	0	2	2
3	2	2	0	3
4	2	2	3	0

Distance Connectivity Matrix

	1	2	3	4
1	6	4	2	2
2	4	6	2	2
3	2	2	1	3
4	2	2	3	1

hydrogen-suppressed matrix

	1	2
1	0	1
2	1	0

	1	2
1	0	4
2	4	0

	1	2
1	6	4
2	4	6

Distance Domination matrix is obtained from the distance matrix $D(G)$ of *G* by replacing the a_{ii} element by 1 if and only if $v_i \in S$. S being the dominating set. For connectivity matrix $a_{ii}=n_i+1$, n_i stands for the atomic number of the atom i and 1 if and only if $v_i \in S$. S being the dominating set.

Table 4: Distance Domination Matrices

non-hydrogen-suppressed matrix

Distance Matrix

	1	2	3	4
1	1	1	1	2
2	1	1	2	1
3	1	2	0	3
4	2	1	3	0

Distance Atom Connectivity Matrix

	1	2	3	4
1	1	4	2	2
2	4	1	2	2
3	2	2	0	3
4	2	2	3	0

Distance Connectivity Matrix

	1	2	3	4
1	7	4	2	2
2	4	7	2	2
3	2	2	1	3
4	2	2	3	1

hydrogen-suppressed matrix

	1	2
1	1	1
2	1	0

	1	2
1	1	4
2	4	0

	1	2
1	7	4
2	4	6

Table 5: Laplace Matrices

non-hydrogen-suppressed matrix

Laplace Matrix

	1	2	3	4
1	2	-1	-1	0
2	-1	2	0	-1
3	-1	0	1	0
4	0	-1	0	1

Laplace Atom Connectivity Matrix

	1	2	3	4
1	2	-3	-1	0
2	-3	2	0	-1
3	-1	0	1	0
4	0	-1	0	1

Laplace Connectivity Matrix

	1	2	3	4
1	-4	-3	-1	0
2	-3	-4	0	-1
3	-1	0	0	0
4	0	-1	0	0

hydrogen-suppressed matrix

	1	2
1	1	-1
2	-1	1

	1	2
1	1	-3
2	-3	1

	1	2
1	-5	-3
2	-3	-5

Table 6: Laplace Domination Matrices

non-hydrogen-suppressed matrix

Laplace Matrix

	1	2	3	4
1	1	-1	-1	0
2	-1	1	0	-1
3	-1	0	1	0
4	0	-1	0	1

Laplace Atom Connectivity Matrix

	1	2	3	4
1	1	-3	-1	0
2	-3	1	0	-1
3	-1	0	1	0
4	0	-1	0	1

Laplace Connectivity Matrix

	1	2	3	4
1	-5	-3	-1	0
2	-3	-5	0	-1
3	-1	0	0	0
4	0	-1	0	0

hydrogen-suppressed matrix

	1	2
1	0	-1
2	-1	1

	1	2
1	0	-3
2	-3	1

	1	2
1	-6	-3
2	-3	-5

Table 7: Laplace Distance Matrix

non-hydrogen-suppressed matrix

Laplace Distance Matrix

	1	2	3	4
1	2	-1	-1	-2
2	-1	2	-2	-1
3	-1	-2	1	-3
4	-2	-1	-3	1

Laplace Distance Atom Connectivity Matrix

	1	2	3	4
1	2	-4	-2	-2
2	-4	2	-2	-2
3	-2	-2	1	-3
4	-2	-2	-3	1

Laplace Distance Connectivity Matrix

	1	2	3	4
1	-4	-4	-2	-2
2	-4	-4	-2	-2
3	-2	-2	0	-3
4	-2	-2	-3	0

hydrogen-suppressed matrix

	1	2
1	1	-1
2	-1	1

	1	2
1	1	-4
2	-4	1

	1	2
1	-5	-4
2	-4	-5

Table 8: Laplace Distance Domination Matrix

non-hydrogen-suppressed matrix

Laplace Distance Matrix

	1	2	3	4
1	1	-1	-1	-2
2	-1	1	-2	-1
3	-1	-2	1	-3
4	-2	-1	-3	1

Laplace Distance Atom Connectivity Matrix

	1	2	3	4
1	1	-4	-2	-2
2	-4	1	-2	-2
3	-2	-2	1	-3
4	-2	-2	-3	1

Laplace Distance Connectivity Matrix

	1	2	3	4
1	-5	-4	-2	-2
2	-4	-5	-2	-2
3	-2	-2	0	-3
4	-2	-2	-3	0

hydrogen-suppressed matrix

	1	2
1	0	-1
2	-1	1

	1	2
1	0	-4
2	-4	1

	1	2
1	-6	-4
2	-4	-5

Table 9: Signless Laplace Matrix

non-hydrogen-suppressed matrix

Signless Laplace Matrix

	1	2	3	4
1	2	1	1	0
2	1	2	0	1
3	1	0	1	0
4	0	1	0	1

Signless Laplace Atom Connectivity Matrix

	1	2	3	4
1	2	3	1	0
2	3	2	0	1
3	1	0	1	0
4	0	1	0	1

Signless Laplace Connectivity Matrix

	1	2	3	4
1	8	3	1	0
2	3	8	0	1
3	1	0	2	0
4	0	1	0	2

hydrogen-suppressed matrix

	1	2
1	1	1
2	1	1

	1	2
1	1	3
2	3	1

	1	2
1	7	3
2	3	7

Table 10: Signless Laplace Domination Matrix

non-hydrogen-suppressed matrix

Signless Laplace Matrix

	1	2	3	4
1	3	1	1	0
2	1	3	0	1
3	1	0	1	0
4	0	1	0	1

Signless Laplace Atom Connectivity Matrix

	1	2	3	4
1	3	3	1	0
2	3	3	0	1
3	1	0	1	0
4	0	1	0	1

Signless Laplace Connectivity Matrix

	1	2	3	4
1	9	3	1	0
2	3	9	0	1
3	1	0	2	0
4	0	1	0	2

hydrogen-suppressed matrix

	1	2
1	2	1
2	1	1

	1	2
1	2	3
2	3	1

	1	2
1	8	3
2	3	7

Table 11: Signless Laplace Distance Matrix

non-hydrogen-suppressed matrix

Signless Laplace Distance Matrix

	1	2	3	4
1	2	1	1	2
2	1	2	2	1
3	1	2	1	3
4	2	1	3	1

Signless Laplace Distance Atom Connectivity Matrix

	1	2	3	4
1	2	4	2	2
2	4	2	2	2
3	2	2	1	3
4	2	2	3	1

Signless Laplace Distance Connectivity Matrix

	1	2	3	4
1	8	4	2	2
2	4	8	2	2
3	2	2	2	3
4	2	2	3	2

hydrogen-suppressed matrix

	1	2
1	1	1
2	1	1

	1	2
1	1	4
2	4	1

	1	2
1	7	4
2	4	7

Table 12: Signless Laplace Distance Domination Matrix

non-hydrogen-suppressed matrix

Signless Laplace Distance Matrix

	1	2	3	4
1	3	1	1	2
2	1	3	2	1
3	1	2	1	3
4	2	1	3	1

Signless Laplace Distance Atom Connectivity Matrix

	1	2	3	4
1	3	4	2	2
2	4	3	2	2
3	2	2	1	3
4	2	2	3	1

Signless Laplace Distance Connectivity Matrix

	1	2	3	4
1	9	4	2	2
2	4	9	2	2
3	2	2	2	3
4	2	2	3	2

hydrogen-suppressed matrix

	1	2
1	2	1
2	1	1

	1	2
1	2	4
2	4	1

	1	2
1	8	4
2	4	7

3.2 Calculations of characteristic polynomial and Eigen values of hydrogen-suppressed matrix and non-hydrogen-suppressed matrix

Hydrogen-suppressed matrix considers only the molecular skeleton without hydrogen atoms. whereas non hydrogen suppressed matrix is the molecular structure considering all the compounds in the structure. The characteristic polynomial, Eigen values and the calculations of various energies defined in sections 3.1 and 3.2 from the datasets are calculated by using some simple MATLAB codes.

4. PRELIMINARY RESULTS

Table 13: The characteristic polynomial, Eigen values and Various Energies of Ethyne - C2H2 – With Hydrogen

1) Graph Energy		
From Adjacency Matrix	From Atom Connectivity Matrix	From Connectivity Matrix
$\lambda^4-3\lambda^2+1=0$ $\lambda=-\frac{1}{2}-\frac{\sqrt{5}}{2},\frac{1}{2}-\frac{\sqrt{5}}{2}$ $-\frac{1}{2}+\frac{\sqrt{5}}{2},\frac{1}{2}+\frac{\sqrt{5}}{2}$ $E=4.472135954995$	${\lambda_A}^4-11{\lambda_A}^2+1=0$ $\lambda_A=-\frac{3}{2}-\frac{\sqrt{13}}{2},\frac{3}{2}-\frac{\sqrt{13}}{2}$ $-\frac{3}{2}+\frac{\sqrt{13}}{2},\frac{3}{2}+\frac{\sqrt{13}}{2}$ $(E)_A=7.21110255$	${\lambda_C}^4-14{\lambda_C}^3+50{\lambda_C}^2$ $-52\lambda_C+16=0$ $\lambda_C=2-\sqrt{2},2+\sqrt{2}$ $5-\sqrt{17},5+\sqrt{17}$ $(E)_C=14$
2) Distance Energy		
From Distance Matrix	From Distance Atom Connectivity Matrix	From Distance Connectivity Matrix
$\mu^4-20\mu^2-32\mu-12=0$ $\mu=-\sqrt{2}-2,\sqrt{2}-2$ $-\sqrt{10}+2,\sqrt{10}+2$ $E_D=10.3245532$	${\mu_A}^4-41{\mu_A}^2-112\mu_A-48=0$ $\mu_A=-4,-3$ $\frac{7}{2}-\frac{\sqrt{65}}{2},\frac{7}{2}+\frac{\sqrt{65}}{2}$ $(E_D)_A=15.0622577$	${\mu_C}^4-14{\mu_C}^3+20{\mu_C}^2$ $+56\mu_C-96=0$ $\mu_C=-2,2,2,12$ $(E_D)_C=18$
3) Laplace Energy		
From Laplace Matrix	From Laplace Atom Connectivity Matrix	From Laplace Connectivity Matrix
$\psi^4-6\psi^3+10\psi^2-4\psi=0$ $\psi=0,2$ $-\sqrt{2}+2,\sqrt{2}+2$ $E_L=6$	${\psi_A}^4-6{\psi_A}^3+2{\psi_A}^2+12\psi_A-8=0$ $\psi_A=3-\sqrt{5},3+\sqrt{5},\sqrt{2},-\sqrt{2}$ $(E_L)_A=8.8284271247$	${\psi_C}^4+8{\psi_C}^3+5{\psi_C}^2-8\psi_C+1=0$ $\psi_C=-\frac{\sqrt{5}}{2}-\frac{1}{2},\frac{\sqrt{5}}{2}-\frac{1}{2},$ $-\frac{\sqrt{53}}{2}-\frac{7}{2},\frac{\sqrt{53}}{2}-\frac{7}{2}$ $(E_L)_C=9.51617786678$
4) Laplace Distance Energy		
From Laplace Distance Matrix	From Laplace Distance Atom Connectivity Matrix	From Laplace Distance Connectivity Matrix
$\beta^4-6\beta^3-7\beta^2+88\beta-121$ $E_{LD}=13.708203932499$	${\beta_A}^4-6{\beta_A}^3-28{\beta_A}^2+216\beta_A-288$ $(E_{LD})_A=18$	${\beta_C}^4+8{\beta_C}^3-25{\beta_C}^2-24\beta_C=0$ $(E_{LD})_C=14$

5) Signless Laplace Energy		
From Signless Laplace Matrix	From Signless Laplace Atom Connectivity Matrix	From Signless Laplace Connectivity Matrix
$q^4-6q^3+10q^2-4q=0$ $E_{SL}=6$	${q_A}^4-6{q_A}^3+2{q_A}^2+12q_A-8=0$ $\left(E_{SL}\right)_A=8.828427124746$	${q_C}^4-20{q_C}^3+121{q_C}^2$ $-264q_C+189=0$ $\left(E_{SL}\right)_C=20$
6) Signless Laplace Distance Energy		
From Signless Laplace Distance Matrix	From Signless Laplace Distance Atom Connectivity Matrix	From Signless Laplace Distance Connectivity Matrix
$\rho^4-6\rho^3-7\rho^2+24\rho-9=0$ $E_{SLD}=10.60555127546$	${\rho_A}^4-6{\rho_A}^3-28{\rho_A}^2-8\rho_A+32=0$ $\left(E_{SLD}\right)_A=14$	${\rho_C}^4-20{\rho_C}^3+91{\rho_C}^2-64\rho_C-176=0$ $\left(E_{SLD}\right)_C=22$
7) Laplacian Energy		
From Laplace Matrix	From Laplace Atom Connectivity Matrix	From Laplace Connectivity Matrix
$\psi^4-6\psi^3+10\psi^2-4\psi=0$ $E_{L_n}=4.828427124746$ $\hat{E}_{L_n}=5.828427$	${\psi_A}^4-6{\psi_A}^3+2{\psi_A}^2+12\psi_A-8=0$ $\left(E_{L_n}\right)_A=7.4721359549995$ $\left(\hat{E}_{L_n}\right)_A=9.47213595$	${\psi_C}^4+8{\psi_C}^3+5{\psi_C}^2-8\psi_C+1=0$ $\left(E_{L_n}\right)_C=14$ $\left(\hat{E}_{L_n}\right)_C=18$
8) Laplacian Distance Energy		
From Laplace Distance Matrix	From Laplace Distance Atom Connectivity Matrix	From Laplace Distance Connectivity Matrix
$\beta^4-6\beta^3-7\beta^2+88\beta-121$ $E_{L_nD}=10.708203932499$ $\hat{E}_{L_nD}=8.9442719$	${\beta_A}^4-6{\beta_A}^3-28{\beta_A}^2+216\beta_A-288$ $\left(E_{L_nD}\right)_A=15$ $\left(\hat{E}_{L_nD}\right)_A=14$	${\beta_C}^4+8{\beta_C}^3-25{\beta_C}^2-24\beta_C=0$ $\left(E_{L_nD}\right)_C=17$ $\left(\hat{E}_{L_nD}\right)_C=19$
9) Signless Laplacian Energy		
From Signless Laplace Matrix	From Signless Laplace Atom Connectivity Matrix	From Signless Laplace Connectivity Matrix
$q^4-6q^3+10q^2-4q=0$ $E_{SL_n}=4.828427124746$ $\hat{E}_{SL_n}=5.8284271$	${q_A}^4-6{q_A}^3+2{q_A}^2+12q_A-8=0$ $\left(E_{SL_n}\right)_A=7.4721359549995$ $\left(\hat{E}_{SL_n}\right)_A=9.472135954999$	${q_C}^4-20{q_C}^3+121{q_C}^2-264q_C+189=0$ $\left(E_{SL_n}\right)_C=14$ $\left(\hat{E}_{SL_n}\right)_C=12.82509573$

10) Signless Laplacian Distance Energy		
From Signless Laplace Distance Matrix	From Signless Laplace Distance Atom Connectivity Matrix	From Signless Laplace Distance Connectivity Matrix
$\rho^4 - 6\rho^3 - 7\rho^2 + 24\rho - 9 = 0$ $E_{SL_nD} = 10.082762530298$ $\hat{E}_{SL_nD} = 12.08276253$	$\rho_A{}^4 - 6\rho_A{}^3 - 28\rho_A{}^2 - 8\rho_A + 32 = 0$ $\left(E_{SL_nD}\right)_A = 15.246211251235$ $\left(\hat{E}_{SL_nD}\right)_A = 17.2462$	$\rho_C{}^4 - 20\rho_C{}^3 + 91\rho_C{}^2 - 64\rho_C - 176 = 0$ $\left(E_{SL_nD}\right)_C = 19$ $\left(\hat{E}_{SL_nD}\right)_C = 17$

Table 14: The characteristic polynomial, Eigen values and Various Domination Energies of Ethyne - C2H2 - With Hydrogen

11) Domination Energy		
From Domination Matrix	From Domination Atom Connectivity Matrix	From Domination Connectivity Matrix
$\kappa^4 - 2\kappa^3 - 2\kappa^2 + 2\kappa + 1 = 0$ $E_\gamma = 4.828427124746$	$\kappa_A{}^4 - 2\kappa_A{}^3 - 10\kappa_A{}^2 + 2\kappa_A + 1 = 0$ $\left(E_\gamma\right)_A = 7.300563079745769$	$\kappa_C{}^4 - 16\kappa_C{}^3 + 67\kappa_C{}^2 - 78\kappa_C + 27 = 0$ $\left(E_\gamma\right)_C = 16$
12) Distance Domination Energy		
From Distance Domination Matrix	From Distance Domination Atom Connectivity Matrix	From Distance Domination Connectivity Matrix
$\sigma^4 - 2\sigma^3 - 19\sigma^2 - 4\sigma + 3 =$ $E_{D_\gamma} = 9.68831380576$	$\sigma_A{}^4 - 2\sigma_A{}^3 - 40\sigma_A{}^2 - 78\sigma_A - 9 =$ $\left(E_{D_\gamma}\right)_A = 14.246211251235$	$\sigma_C{}^4 - 16\sigma_C{}^3 + 37\sigma_C{}^2 + 62\sigma_C - 168 = 0$ $\left(E_{D_\gamma}\right)_C = 20$
13) Laplace Domination Energy		
From Laplace Domination Matrix	From Laplace Domination Atom Connectivity Matrix	From Laplace Domination Connectivity Matrix
$\alpha^4 - 4\alpha^3 + 3\alpha^2 + 2\alpha - 1 = 0$ $E_{L_\gamma} = 5.2360679774$	$\alpha_A{}^4 - 4\alpha_A{}^3 - 5\alpha_A{}^2 + 18\alpha_A - 9 = 0$ $\left(E_{L_\gamma}\right)_A = 8.6055512754$	$\alpha_C{}^4 + 10\alpha_C{}^3 + 14\alpha_C{}^2 - 10\alpha_C + 1 = 0$ $\left(E_{L_\gamma}\right)_C = 11.07463837598$
14) Laplace Distance Domination Energy		
From Laplace Distance Domination Matrix	From Laplace Distance Domination Atom Connectivity Matrix	From Laplace Distance Domination Connectivity Matrix
$\phi^4 - 4\phi^3 - 14\phi^2 + 68\phi - 63 =$ $E_{LD_\gamma} = 12.32455532$	$\phi_A{}^4 - 4\phi_A{}^3 - 35\phi_A{}^2 + 190\phi_A - 200 =$ $\left(E_{LD_\gamma}\right)_A = 17.062257748$	$\phi_C{}^4 + 10\phi_C{}^3 - 16\phi_C{}^2 - 58\phi_C - 33 = 0$ $\left(E_{LD_\gamma}\right)_C = 16$

15) Signless Laplace Domination Energy		
From Signless Laplace Domination Matrix	From Signless Laplace Domination Atom Connectivity Matrix	From Signless Laplace Domination Connectivity Matrix
$\delta^4 - 8\delta^3 + 19\delta^2 - 14\delta + 3 =$ $E_{SL_\gamma} = 8$	$\delta_A{}^4 - 8\delta_A{}^3 + 11\delta_A{}^2 + 2\delta_A - 5 = 0$ $\left(E_{SL_\gamma}\right)_A = 9.2360679774$	$\delta_C{}^4 - 22\delta_C{}^3 + 146\delta_C{}^2 - 338\delta_C + 253 = 0$ $\left(E_{SL_\gamma}\right)_C = 22$
16) Signless Laplace Distance Domination Energy		
From Signless Laplace Distance Domination Matrix	From Signless Laplace Distance Domination Atom Connectivity Matrix	From Signless Laplace Distance Domination Connectivity Matrix
$\eta^4 - 8\eta^3 + 2\eta^2 + 40\eta - 35 =$ $E_{SLD_\gamma} = 12.47213595$	$\eta_A{}^4 - 8\eta_A{}^3 - 19\eta_A{}^2 + 14\eta_A + 24 = 0$ $\left(E_{SLD_\gamma}\right)_A = 14$	$\eta_C{}^4 - 22\eta_C{}^3 + 116\eta_C{}^2 - 106\eta_C - 245 = 0$ $\left(E_{SLD_\gamma}\right)_C = 24$
17) Laplacian Domination Energy		
From Laplace Domination Matrix	From Laplace Domination Atom Connectivity Matrix	From Laplace Domination Connectivity Matrix
$\alpha^4 - 4\alpha^3 + 3\alpha^2 + 2\alpha - 1 = 0$ $\left(E_{L_{n\gamma}}\right) = 4.4721359549995$ $\left(\hat{E}_{L_{n\gamma}}\right) = 6.236067977$	$\alpha_A{}^4 - 4\alpha_A{}^3 - 5\alpha_A{}^2 + 18\alpha_A - 9 = 0$ $\left(E_{L_{n\gamma}}\right)_A = \sqrt{13} + 4 = 7.605551275$ $\left(\hat{E}_{L_{n\gamma}}\right)_A = \sqrt{13} + 6 = 9.605551275$	$\alpha_C{}^4 + 10\alpha_C{}^3 + 14\alpha_C{}^2 - 10\alpha_C + 1 = 0$ $\left(E_{L_{n\gamma}}\right)_C = 16$ $\left(\hat{E}_{L_{n\gamma}}\right)_C = 20$
18) Laplacian Distance Domination Energy		
From Laplace Distance Domination Matrix	From Laplace Distance Domination Atom Connectivity Matrix	From Laplace Distance Domination Connectivity Matrix
$\phi^4 - 4\phi^3 - 14\phi^2 + 68\phi - 63 =$ $E_{L_nD_\gamma} = 9.32455532$ $\hat{E}_{L_nD_\gamma} = 9.828427$	$\phi_A{}^4 - 4\phi_A{}^3 - 35\phi_A{}^2 + 190\phi_A - 200 =$ $\left(E_{L_nD_\gamma}\right)_A = 14.062257748$ $\left(\hat{E}_{L_nD_\gamma}\right)_A = 14$	$\phi_C{}^4 + 10\phi_C{}^3 - 16\phi_C{}^2 - 58\phi_C - 33 = 0$ $\left(E_{L_nD_\gamma}\right)_C = 19$ $\left(\hat{E}_{L_nD_\gamma}\right)_C = 21$
19) Signless Laplacian Domination Energy		
From Signless Laplace Domination Matrix	From Signless Laplace Domination Atom Connectivity Matrix	From Signless Laplace Domination Connectivity Matrix

$\delta^4-8\delta^3+19\delta^2-14\delta+3=$ $E_{SL_{n\gamma}}=5.84161925296$ $\hat{E}_{SL_{n\gamma}}=5.84161925296$	${\delta_A}^4-8{\delta_A}^3+11{\delta_A}^2+2\delta_A-5=0$ $\left(E_{SL_{n\gamma}}\right)_A=7.6212327846$ $\left(\hat{E}_{SL_{n\gamma}}\right)_A=9.385164807$	${\delta_C}^4-22{\delta_C}^3+146{\delta_C}^2-338\delta_C+253=0$ $\left(E_{SL_{n\gamma}}\right)_C=16$ $\left(\hat{E}_{SL_{n\gamma}}\right)_C=14.67017498$
20) Signless Laplacian Distance Domination Energy		
From Signless Laplace Distance Domination Matrix	From Signless Laplace Distance Domination Atom Connectivity Matrix	From Signless Laplace Distance Domination Connectivity Matrix
$\eta^4-8\eta^3+2\eta^2+40\eta-35=$ $E_{SL_nD_\gamma}=10.472135954$ $\hat{E}_{SL_nD_\gamma}=11$	${\eta_A}^4-8{\eta_A}^3-19{\eta_A}^2+14\eta_A+24=0$ $\left(E_{SL_nD_\gamma}\right)_A=14.544003745$ $\left(\hat{E}_{SL_nD_\gamma}\right)_A=16.544003745$	${\eta_C}^4-22{\eta_C}^3+116{\eta_C}^2-106\eta_C-245=0$ $\left(E_{SL_nD_\gamma}\right)_C=21$ $\left(\hat{E}_{SL_nD_\gamma}\right)_C=19$

Table 15: The characteristic polynomial, Eigen values and Various Energies of Ethyne - C2H2 – Without Hydrogen

Various Energies	Adjacency Matrix	Atom Connectivity Matrix	Connectivity Matrix
Graph Energy	$\lambda^2-1=0$ $E=2$	${\lambda_A}^2-9=0$ $\left(E\right)_A=6$	${\lambda_C}^2-12\lambda_C+27=0$ $\left(E\right)_C=12$
Distance Energy	$\mu^2-1=0$ $E_D=2$	${\mu_A}^2-16=0$ $\left(E_D\right)_A=8$	${\mu_C}^2-12\mu_C+20=0$ $\left(E_D\right)_C=12$
Laplace Energy	$\psi^2-2\psi=0$ $E_L=2$	${\psi_A}^2-2\psi_A-8=0$ $\left(E_L\right)_A=6$	${\psi_C}^2+10\psi_C+16=0$ $\left(E_L\right)_C=10$
Laplace Distance Energy	$\beta^2-2\beta=0$ $E_{LD}=2$	${\beta_A}^2-2\beta_A-15=0$ $\left(E_{LD}\right)_A=8$	${\beta_C}^2+10\beta_C+9=0$ $\left(E_{LD}\right)_C=10$
Signless Laplace Energy	$q^2-2q=0$ $E_{SL}=2$	${q_A}^2-2q_A-8=0$ $\left(E_{SL}\right)_A=6$	${q_C}^2-14q_C+40=0$ $\left(E_{SL}\right)_C=14$
Signless Laplace Distance Energy	$\rho^2-2\rho=0$ $E_{SLD}=2$	${\rho_A}^2-2\rho_A-15=0$ $\left(E_{SLD}\right)_A=8$	${\rho_C}^2-14\rho_C+33=0$ $\left(E_{SLD}\right)_C=14$
Laplacian Energy	$\psi^2-2\psi=0$ $E_{L_n}=2$ $\hat{E}_{L_n}=4$	${\psi_A}^2-2\psi_A-8=0$ $\left(E_{L_n}\right)_A=6$ $\left(\hat{E}_{L_n}\right)_A=6$	${\psi_C}^2+10\psi_C+16=0$ $\left(E_{L_n}\right)_C=12$ $\left(\hat{E}_{L_n}\right)_C=16$

Laplacian Distance Energy	$\beta^2 - 2\beta = 0$ $E_{L_nD} = 2$ $\hat{E}_{L_nD} = 4$	${\beta_A}^2 - 2\beta_A - 15 = 0$ $\left(E_{L_nD}\right)_A = 8$ $\left(\hat{E}_{L_nD}\right)_A = 8$	${\beta_C}^2 + 10\beta_C + 9 = 0$ $\left(E_{L_nD}\right)_C = 12$ $\left(\hat{E}_{L_nD}\right)_C = 16$
Signless Laplacian Energy	$q^2 - 2q = 0$ $E_{SL_n} = 2$ $\hat{E}_{SL_n} = 4$	${q_A}^2 - 2q_A - 8 = 0$ $\left(E_{SL_n}\right)_A = 6$ $\left(\hat{E}_{SL_n}\right)_A = 6$	${q_C}^2 - 14q_C + 40 = 0$ $\left(E_{SL_n}\right)_C = 12$ $\left(\hat{E}_{SL_n}\right)_C = 8$
Signless Laplacian Distance Energy	$\rho^2 - 2\rho = 0$ $E_{SL_nD} = 2$ $\hat{E}_{SL_nD} = 4$	${\rho_A}^2 - 2\rho_A - 15 = 0$ $\left(E_{SL_nD}\right)_A = 8$ $\left(\hat{E}_{SL_nD}\right)_A = 8$	${\rho_C}^2 - 14\rho_C + 33 = 0$ $\left(E_{SL_nD}\right)_C = 12$ $\left(\hat{E}_{SL_nD}\right)_C = 8$

Table 16: The characteristic polynomial, Eigen values and Various Domination Energies of Ethyne - C2H2 - Without Hydrogen

Domination Energy	$\kappa^2 - \kappa - 1 = 0$ $E_\gamma = 2.236067977$	${\kappa_A}^2 - \kappa_A - 9 = 0$ $\left(E_\gamma\right)_A = 6.082762530298$	${\kappa_C}^2 - 13\kappa_C + 33 = 0$ $\left(E_\gamma\right)_C = 13$
Distance Domination Energy	$\sigma^2 - \sigma - 1 = 0$ $E_{D_\gamma} = 2.236067977$	${\sigma_A}^2 - \sigma_A - 16 = 0$ $\left(E_{D_\gamma}\right)_A = 8.0622577$	${\sigma_C}^2 - 13\sigma_C + 26 = 0$ $\left(E_{D_\gamma}\right)_C = 13$
Laplace Domination Energy	$\alpha^2 - \alpha - 1 = 0$ $E_{L_\gamma} = 2.23606$	${\alpha_A}^2 - \alpha_A - 9 = 0$ $\left(E_{L_\gamma}\right)_A = 6.0827625$	${\alpha_C}^2 + 11\alpha_C + 21 = 0$ $\left(E_{L_\gamma}\right)_C = 11$
Laplace Distance Domination Energy	$\phi^2 - \phi - 1 = 0$ $E_{LD_\gamma} = 2.23606$	${\phi_A}^2 - \phi_A - 16 = 0$ $\left(E_{LD_\gamma}\right)_A = 8.06225$	${\phi_C}^2 + 11\phi_C + 14 = 0$ $\left(E_{LD_\gamma}\right)_C = 11$
Signless Laplace Domination Energy	$\delta^2 - 3\delta + 1 = 0$ $E_{SL_\gamma} = 3$	${\delta_A}^2 - 3\delta_A - 7 = 0$ $\left(E_{SL_\gamma}\right)_A = 6.08276$	${\delta_C}^2 - 15\delta_C + 47 = 0$ $\left(E_{SL_\gamma}\right)_C = 15$
Signless Laplace Distance Domination Energy	$\eta^2 - 3\eta + 1 = 0$ $E_{SLD_\gamma} = 3$	${\eta_A}^2 - 3\eta_A - 14 = 0$ $\left(E_{SLD_\gamma}\right)_A = 8.06225$	${\eta_C}^2 - 15\eta_C + 40 = 0$ $\left(E_{SLD_\gamma}\right)_C = 15$
Laplacian Domination Energy	$\alpha^2 - \alpha - 1 = 0$ $\left(E_{L_{n\gamma}}\right) = 2.236067977$ $\left(\hat{E}_{L_{n\gamma}}\right) = 5$	${\alpha_A}^2 - \alpha_A - 9 = 0$ $\left(E_{L_{n\gamma}}\right)_A = 6.082762$ $\left(\hat{E}_{L_{n\gamma}}\right)_A = 6.082762$	${\alpha_C}^2 + 11\alpha_C + 21 = 0$ $\left(E_{L_{n\gamma}}\right)_C = 13$ $\left(\hat{E}_{L_{n\gamma}}\right)_C = 17$

Laplacian Distance Domination Energy	$\phi^2-\phi-1=0$ $E_{L_nD_\gamma}=2.23606$ $\widehat{E}_{L_nD_\gamma}=5$	${\phi_A}^2-\phi_A-16=0$ $\left(E_{L_nD_\gamma}\right)_A=8.06225$ $\left(\widehat{E}_{L_nD_\gamma}\right)_A=8.06225$	${\phi_C}^2+11\phi_C+14=0$ $\left(E_{L_nD_\gamma}\right)_C=13$ $\left(\widehat{E}_{L_nD_\gamma}\right)_C=17$
Signless Laplacian Domination Energy	$\delta^2-3\delta+1=0$ $E_{SL_{n\gamma}}=2.236067977$ $\widehat{E}_{SL_{n\gamma}}=3$	${\delta_A}^2-3\delta_A-7=0$ $\left(E_{SL_{n\gamma}}\right)_A=6.08276$ $\left(\widehat{E}_{SL_{n\gamma}}\right)_A=6.08276$	${\delta_C}^2-15\delta_C+47=0$ $\left(E_{SL_{n\gamma}}\right)_C=13$ $\left(\widehat{E}_{SL_{n\gamma}}\right)_C=9$
Signless Laplacian Distance Domination Energy	$\eta^2-3\eta+1=0$ $E_{SL_nD_\gamma}=2.2360679$ $\widehat{E}_{SL_nD_\gamma}=3$	${\eta_A}^2-3\eta_A-14=0$ $\left(E_{SL_nD_\gamma}\right)_A=8.062257$ $\left(\widehat{E}_{SL_nD_\gamma}\right)_A=8.062257$	${\eta_C}^2-15\eta_C+40=0$ $\left(E_{SL_nD_\gamma}\right)_C=13$ $\left(\widehat{E}_{SL_nD_\gamma}\right)_C=9$

5. BOUNDS OF DOMINATION IN GRAPHS

In the below bounds, $|S|$ is the cardinality of the set considered for finding the set energy. whereas in the atom connectivity and connectivity matrices, $|S|$ is considered as atomic number of the molecule in case of connectivity matrices. Moreover, without loss of generality except Laplace and Laplace distance energies, it can be noted that energy obtained from adjacency matrix $\leq$ energy obtained from atom connectivity matrices matrix $\leq$ energy obtained from connectivity matrices matrix

Theorem. Let $G \neq K_n$, $n \geq 3$. Then, $\sqrt{2m+|S|+n(n-1)(\det A)^{2/n}} \leq E_{\gamma-Min}(G) \leq \sqrt{(2m+|S|)n}$.

Proof: Let the Eigen values of *G* be $\kappa_1, \kappa_2, \kappa_3, \ldots\ldots, \kappa_n$ corresponding to the minimal dominating set. By the definition of domination energy we have, $E_{\gamma-Min}(G)=\sum_{i=1}^{n}|\kappa_i|$.

$$\left(E_{\gamma-Min}(G)\right)^2=\left(\sum_{i=1}^{n}|\kappa_i|\right)^2=\sum_{i=1}^{n}{\kappa_i}^2+2\sum_{i\neq j}|\kappa_i||\kappa_j|.$$

The arithmetic mean of a set of positive number is greater than or equal to their geometric mean, we have.

$$\frac{1}{n(n-1)}\sum_{i\neq j}|\kappa_i||\kappa_j|\geq\left(\prod_{i\neq j}|\kappa_i||\kappa_j|\right)^{\frac{2}{n(n-1)}}$$

$$\left(\prod_{i=1}^{n}|\kappa_i|^{2(n-1)}\right)^{\frac{1}{n(n-1)}}=\left(\prod_{i=1}^{n}|\kappa_i|\right)^{\frac{2}{n}}=(\det A)^{\frac{2}{n}}$$

Using $\sum_{i=1}^{n}(\kappa_i)^2=2m+|S|$,

We obtain $\left(E_{\gamma-Min}(G)\right)^2 \geq 2m+|S|+n(n-1)(\det A)^{2/n}\right)$

Therefore, lower bound holds.

To prove the other inequality, we apply Holder's inequality to the two vectors in R^n,

$u = \left(|\kappa_1|, |\kappa_2|, ..., |\kappa_n|\right)$ and $v = (1,1,.....,1)$.

This gives

$$\sum_{i=1}^{n} |\kappa_i| \le \sqrt{\sum_{i=1}^{n} \kappa_i^{\,2}}\sqrt{n} \le \sqrt{(2m + |S|)n},$$

Therefore, upper bound holds. Hence proved. □

6. OPEN PROBLEM

- Study of atom connectivity and connectivity energy for other compounds.
- Find the significance of these energies with respect to the physical properties of the compound.
- Compare energies and atom connectivity and connectivity energies of different compounds and characterize them.
- Finding the relationship between the structure of a compound and the energy of the compound.

7. CONCLUSION

The purpose of this study is to investigate the various energy of graph through the new perspective of atom connectivity matrix and connectivity matrix. The current study is innovative, and this approach has not yet been studied. Moreover, the new study will explore the various possible applications in the field of applied sciences.

In this paper we introduced the various energy of graph through atom connectivity matrix (ACM) and in general connectivity matrix (CM). In the previous studies the significance of double bond, triple bond or atoms are not properly interpreted in energy of graph. Here we are defined the various energies by considering the types of the bonds in the molecule and the significant of double bond, triple bond or atomic number are interpreted in energy of graph. Calculations of characteristic polynomial and Eigen values, various energies from the hydrogen-suppressed matrix and non-hydrogen-suppressed matrix are calculated in the compound Ethyne - C2H2.

In future works, the significance of these energies with respect to the physical properties of the compounds need to be developed. The various results, theorem related to the atom connectivity and connectivity energies in new perspective are to include in future works.

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