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Atom Connectivity and Connectivity Energy of few Molecules

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ABSTRACT: For a given chemical compound, a molecular graph could be constructed. The total of the absolute measures of Eigen values taken from adjacency matrix of the molecular graph for the assumed chemical compound is known as the energy of graph. It has been observed that, the adjacency matrix derived from the molecular graph has no information about the atoms and bonds connected. To overcome this limitation, we have considered the atom-connectivity and connectivity matrix which give more information about the classification of bonds and atom-connectivity of a chemical compound in the molecular graph. In this paper, we enhance our results on the atom connectivity energy graph and also few hydrocarbons are compared with the ordinary energy.

1. INTRODUCTION

The theory of energy graph is developed in industrial chemistry, where specific numerical quantities (as the heat generation of hydrocarbon graph) are associated to total electron-energy, which can be evaluated as the energy of respective molecular graph. The molecular graph is the representation of molecular structure of a hydrocarbon molecule whose vertices are the position of carbon atoms and two vertices are adjacent, if there is a bond joining them. Eigen values and Eigen vectors provide the insights into the geometry of the related linear transformation. The energy of the graph is the total-sum of the absolute measure of the Eigenvalues of the corresponding adjacency matrix. Through the great work of Coulson [3], many researchers had continuous interest towards the general mathematical characteristics of the total pi-electron energy (E), evaluated within the framework of Huckel Molecular Orbital (HMO) model. Because of all these efforts many scientists could get an insight into the dependence of "E" on molecular structure. The characteristics of energy "E" (pi electron energy) are elaborated by many authors [1-4, 8-10].

The energy so obtained represents the physical/chemical features of the molecules. The above mentioned concept of 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) [24,25, 33-35].

The main purpose of this research is to analyze 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 in the field of energy or graph. Moreover, the new study will explore the various possible applications in the field of applied sciences.

2. PROBLEM STATEMENT

It has been observed that, the adjacency matrix derived from the molecular graph has no information about the atoms and bonds connecting the atoms.

In order to overcome this limitation, we have considered the atom-connectivity and connectivity matrix which give more information about the classification of bonds and atom- connectivity of a chemical compound in the molecular graph. The application of atom-connectivity and connectivity matrix in energy of graph will help to understand the physical and chemical properties of the compound with respect to the structure of the compound.

3. BACKGROUND

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 [8]. 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 [32-34]. 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. Various researchers have obtained extensive results with respect to energy of graph [5, 11-18, 26-29, 36].

The lists of few familiar energies of graph are given as below [19-23]. 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 explore the molecule on the computer screen, the molecular structure details should be taken as input to the system. Molecular modeling software needs this information to be provided in the form of a graph 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 [1] for computer representation of molecules, Spialter [31-33] introduced the concept of atom connectivity matrix. Mathavi Manisekar and S. Lalitha have also obtained few results in Dissociation Energy for Amino Acids [30].

The atom-connectivity matrix, denoted by ACM, has been proposed by Spialter [31-33] for the use in computer-oriented chemical nomenclature. This matrix represents the structural formula of a molecule and is given by

$$[ACM]_{ij} = \begin{cases} b_{ij} & \text{if vertices } i \text{ and } j \text{ are adjacent} \\ s_i & \text{if } i = j \\ 0 & \text{otherwise} \end{cases} \quad (1)$$

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 for single, 1.5 for aromatic, 2 for double and 3 triple bonds. 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 [31-33]. 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.

$$[CM]_{ij} = \begin{cases} b_{ij} & \text{if vertices } i \text{ and } j \text{ are adjacent} \\ n_i & \text{if } i = j \\ 0 & \text{otherwise} \end{cases} \quad (2)$$

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

4. MATERIALS AND METHODS

4.1. Definitions

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

$$E = E(G) = \sum_{i=1}^{n} |\lambda_i| \qquad (3)$$

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 : $A(G)$. Domination Energy of Graph [6] : $E_\gamma = E_\gamma(G) = \sum_{i=1}^{n} |\kappa_i| \qquad (4)$

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 : $A_\gamma(G)$

4.1.1. Minimal domination energy

A dominating set D in G is a minimal dominating set if no proper subset of D is a dominating set. The domination energy $E_\gamma(G)$ obtained for a minimal dominating set is called the minimal domination energy denoted by $E_{\gamma-Min}(G)$.

4.1.2 Maximal domination energy.

A dominating set D in G is a maximal dominating set if D contains all the vertices of G. The domination energy $E_\gamma(G)$ obtained for a maximal dominating set is called the maximal domination energy denoted by $E_{\gamma-Max}(G)$.

Similar to the above definitions all energies could be defined in a similar way. For all definitions kindly refer to [7,19-25]

4.2. Main Results

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 and 2. Let us take an example of Benzene

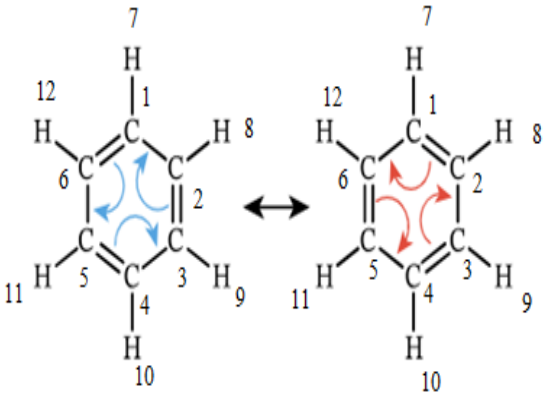

Figure 1: Non hydrogen-suppressed Benzene molecule

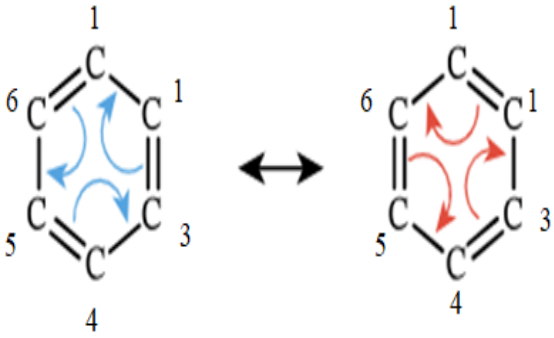

Figure 2: Hydrogen-suppressed Benzene molecule

Adjacency Matrix With Hydrogen

	1	2	3	4	5	6	7	8	9	10	11	12
1	0	1	0	0	0	1	1	0	0	0	0	0
2	1	0	1	0	0	0	0	1	0	0	0	0
3	0	1	0	1	0	0	0	0	1	0	0	0
4	0	0	1	0	1	0	0	0	0	1	0	0
5	0	0	0	1	0	1	0	0	0	0	1	0
6	1	0	0	0	1	0	0	0	0	0	0	1
7	1	0	0	0	0	0	0	0	0	0	0	0
8	0	1	0	0	0	0	0	0	0	0	0	0
9	0	0	1	0	0	0	0	0	0	0	0	0
10	0	0	0	1	0	0	0	0	0	0	0	0
11	0	0	0	0	1	0	0	0	0	0	0	0
12	0	0	0	0	0	1	0	0	0	0	0	0

Adjacency Matrix Without Hydrogen

	1	2	3	4	5	6
1	0	1	0	0	0	1
2	1	0	1	0	0	0
3	0	1	0	1	0	0
4	0	0	1	0	1	0
5	0	0	0	1	0	1
6	1	0	0	0	1	0

Atom Connectivity Matrix With Hydrogen

	1	2	3	4	5	6	7	8	9	10	11	12
1	C	1	0	0	0	2	1	0	0	0	0	0
2	1	C	2	0	0	0	0	1	0	0	0	0
3	0	2	C	1	0	0	0	0	1	0	0	0
4	0	0	1	C	2	0	0	0	0	1	0	0
5	0	0	0	2	C	1	0	0	0	0	1	0
6	2	0	0	0	1	C	0	0	0	0	0	1
7	1	0	0	0	0	0	H	0	0	0	0	0
8	0	1	0	0	0	0	0	H	0	0	0	0
9	0	0	1	0	0	0	0	0	H	0	0	0
10	0	0	0	1	0	0	0	0	0	H	0	0
11	0	0	0	0	1	0	0	0	0	0	H	0
12	0	0	0	0	0	1	0	0	0	0	0	H

Isomorphic Graph (Isomers)

	1	2	3	4	5	6	7	8	9	10	11	12
1	C	2	0	0	0	1	1	0	0	0	0	0
2	2	C	1	0	0	0	0	1	0	0	0	0
3	0	1	C	2	0	0	0	0	1	0	0	0
4	0	0	2	C	1	0	0	0	0	1	0	0
5	0	0	0	1	C	2	0	0	0	0	1	0
6	1	0	0	0	2	C	0	0	0	0	0	1
7	1	0	0	0	0	0	H	0	0	0	0	0
8	0	1	0	0	0	0	0	H	0	0	0	0
9	0	0	1	0	0	0	0	0	H	0	0	0
10	0	0	0	1	0	0	0	0	0	H	0	0
11	0	0	0	0	1	0	0	0	0	0	H	0
12	0	0	0	0	0	1	0	0	0	0	0	H

Atom Connectivity Matrix Without Hydrogen

	1	2	3	4	5	6
1	C	1	0	0	0	2
2	1	C	2	0	0	0
3	0	2	C	1	0	0
4	0	0	1	C	2	0
5	0	0	0	2	C	1
6	2	0	0	0	1	C

Connectivity Matrix Without Hydrogen

	1	2	3	4	5	6
1	6	1	0	0	0	2
2	1	6	2	0	0	0
3	0	2	6	1	0	0
4	0	0	1	6	2	0
5	0	0	0	2	6	1
6	2	0	0	0	1	6

Isomorphic Graph (Isomers)

	1	2	3	4	5	6
1	C	2	0	0	0	1
2	2	C	1	0	0	0
3	0	1	C	2	0	0
4	0	0	2	C	1	0
5	0	0	0	1	C	2
6	1	0	0	0	2	C

The above matrices define the various kindly of atom connectivity and connectivity matrices with respect to the benezene compound.

Connectivity Matrix With Hydrogen

	1	2	3	4	5	6	7	8	9	10	11	12
1	6	1	0	0	0	2	1	0	0	0	0	0
2	1	6	2	0	0	0	0	1	0	0	0	0
3	0	2	6	1	0	0	0	0	1	0	0	0
4	0	0	1	6	2	0	0	0	0	1	0	0
5	0	0	0	2	6	1	0	0	0	0	1	0
6	2	0	0	0	1	6	0	0	0	0	0	1
7	1	0	0	0	0	0	1	0	0	0	0	0
8	0	1	0	0	0	0	0	1	0	0	0	0
9	0	0	1	0	0	0	0	0	1	0	0	0
10	0	0	0	1	0	0	0	0	0	1	0	0
11	0	0	0	0	1	0	0	0	0	0	1	0
12	0	0	0	0	0	1	0	0	0	0	0	1

Isomorphic Graph (Isomers)

	1	2	3	4	5	6	7	8	9	10	11	12
1	6	2	0	0	0	1	1	0	0	0	0	0
2	2	6	1	0	0	0	0	1	0	0	0	0
3	0	1	6	2	0	0	0	0	1	0	0	0
4	0	0	2	6	1	0	0	0	0	1	0	0
5	0	0	0	1	6	2	0	0	0	0	1	0
6	1	0	0	0	2	6	0	0	0	0	0	1
7	1	0	0	0	0	0	1	0	0	0	0	0
8	0	1	0	0	0	0	0	1	0	0	0	0
9	0	0	1	0	0	0	0	0	1	0	0	0
10	0	0	0	1	0	0	0	0	0	1	0	0
11	0	0	0	0	1	0	0	0	0	0	1	0
12	0	0	0	0	0	1	0	0	0	0	0	1

Isomorphic is same in adjacent matrix (Isomers)

	1	2	3	4	5	6
1	6	2	0	0	0	1
2	2	6	1	0	0	0
3	0	1	6	2	0	0
4	0	0	2	6	1	0
5	0	0	0	1	6	2
6	1	0	0	0	2	6

From the definition of the eigenvector v corresponding to the eigenvalue λ we have $Av = \lambda v$, then $(A-\lambda I)v = 0$, $\det(A-\lambda I)v = 0$. The characteristic polynomial for Adjacency Matrix With Hydrogen is given as

$$\lambda^{12} - 12\lambda^{10} + 48\lambda^{8} - 78\lambda^{6} + 48\lambda^{4} - 12\lambda^{2} + 1 = 0 \qquad (5)$$

Eigenvalues are given as below

$$\lambda_1 = \frac{\sqrt{5}-1}{2} = 0.6180, \lambda_2 = \frac{-\sqrt{5}+1}{2} = -0.6180,$$

$$\lambda_3 = \frac{\sqrt{5}+1}{2} = 1.6180, \lambda_4 = \frac{-\sqrt{5}-1}{2} = -1.6180,$$

$$\lambda_5 = \frac{\sqrt{5}-1}{2} = 0.6180, \lambda_6 = \frac{-\sqrt{5}+1}{2} = -0.6180,$$

$$\lambda_7 = \frac{\sqrt{5}+1}{2} = 1.6180, \lambda_8 = \frac{-\sqrt{5}-1}{2} = -1.6180,$$

$$\lambda_9 = \sqrt{2}-1 = 0.4142, \lambda_{10} = -\sqrt{2}+1 = -0.4142,$$

$$\lambda_{11} = \sqrt{2}+1 = 2.4142, \lambda_{12} = -\sqrt{2}-1 = -2.4142.$$

Domination Matrix With Hydrogen

	1	2	3	4	5	6	7	8	9	10	11	12
1	1	1	0	0	0	1	1	0	0	0	0	0
2	1	0	1	0	0	0	0	1	0	0	0	0
3	0	1	0	1	0	0	0	0	1	0	0	0
4	0	0	1	1	1	0	0	0	0	1	0	0
5	0	0	0	1	0	1	0	0	0	0	1	0
6	1	0	0	0	1	0	0	0	0	0	0	1
7	1	0	0	0	0	0	0	0	0	0	0	0
8	0	1	0	0	0	0	0	0	0	0	0	0
9	0	0	1	0	0	0	0	0	0	0	0	0
10	0	0	0	1	0	0	0	0	0	0	0	0
11	0	0	0	0	1	0	0	0	0	0	0	0
12	0	0	0	0	0	1	0	0	0	0	0	0

Domination Matrix Without Hydrogen

	1	2	3	4	5	6
1	1	1	0	0	0	1
2	1	0	1	0	0	0
3	0	1	0	1	0	0
4	0	0	1	1	1	0
5	0	0	0	1	0	1
6	1	0	0	0	1	0

Atom Connectivity Matrix Without Hydrogen

	1	2	3	4	5	6
1	1	1	0	0	0	2
2	1	0	2	0	0	0
3	0	2	0	1	0	0
4	0	0	1	1	2	0
5	0	0	0	2	0	1
6	2	0	0	0	1	0

Atom Connectivity Matrix With Hydrogen

	1	2	3	4	5	6	7	8	9	10	11	12
1	1	1	0	0	0	2	1	0	0	0	0	0
2	1	0	2	0	0	0	0	1	0	0	0	0
3	0	2	0	1	0	0	0	0	1	0	0	0
4	0	0	1	1	2	0	0	0	0	1	0	0
5	0	0	0	2	0	1	0	0	0	0	1	0
6	2	0	0	0	1	0	0	0	0	0	0	1
7	1	0	0	0	0	0	0	0	0	0	0	0
8	0	1	0	0	0	0	0	0	0	0	0	0
9	0	0	1	0	0	0	0	0	0	0	0	0
10	0	0	0	1	0	0	0	0	0	0	0	0
11	0	0	0	0	1	0	0	0	0	0	0	0
12	0	0	0	0	0	1	0	0	0	0	0	0

Isomorphic Graph (Isomers)

	1	2	3	4	5	6	7	8	9	10	11	12
1	1	2	0	0	0	1	1	0	0	0	0	0
2	2	0	1	0	0	0	0	1	0	0	0	0
3	0	1	0	2	0	0	0	0	1	0	0	0
4	0	0	2	1	1	0	0	0	0	1	0	0
5	0	0	0	1	0	2	0	0	0	0	1	0
6	1	0	0	0	2	0	0	0	0	0	0	1
7	1	0	0	0	0	0	0	0	0	0	0	0
8	0	1	0	0	0	0	0	0	0	0	0	0
9	0	0	1	0	0	0	0	0	0	0	0	0
10	0	0	0	1	0	0	0	0	0	0	0	0
11	0	0	0	0	1	0	0	0	0	0	0	0
12	0	0	0	0	0	1	0	0	0	0	0	0

Connectivity Matrix With Hydrogen

	1	2	3	4	5	6	7	8	9	10	11	12
1	7	1	0	0	0	2	1	0	0	0	0	0
2	1	6	2	0	0	0	0	1	0	0	0	0
3	0	2	6	1	0	0	0	0	1	0	0	0
4	0	0	1	7	2	0	0	0	0	1	0	0
5	0	0	0	2	6	1	0	0	0	0	1	0
6	2	0	0	0	1	6	0	0	0	0	0	1
7	1	0	0	0	0	0	1	0	0	0	0	0
8	0	1	0	0	0	0	0	1	0	0	0	0
9	0	0	1	0	0	0	0	0	1	0	0	0
10	0	0	0	1	0	0	0	0	0	1	0	0
11	0	0	0	0	1	0	0	0	0	0	1	0
12	0	0	0	0	0	1	0	0	0	0	0	1

Isomorphic Graph (Isomers)

	1	2	3	4	5	6
1	1	2	0	0	0	1
2	2	0	1	0	0	0
3	0	1	0	2	0	0
4	0	0	2	1	1	0
5	0	0	0	1	0	2
6	1	0	0	0	2	0

Isomorphic Graph (Isomers)

	1	2	3	4	5	6	7	8	9	10	11	12
1	7	2	0	0	0	1	1	0	0	0	0	0
2	2	6	1	0	0	0	0	1	0	0	0	0
3	0	1	6	2	0	0	0	0	1	0	0	0
4	0	0	2	7	1	0	0	0	0	1	0	0
5	0	0	0	1	6	2	0	0	0	0	1	0
6	1	0	0	0	2	6	0	0	0	0	0	1
7	1	0	0	0	0	0	1	0	0	0	0	0
8	0	1	0	0	0	0	0	1	0	0	0	0
9	0	0	1	0	0	0	0	0	1	0	0	0
10	0	0	0	1	0	0	0	0	0	1	0	0
11	0	0	0	0	1	0	0	0	0	0	1	0
12	0	0	0	0	0	1	0	0	0	0	0	1

Connectivity Matrix Without Hydrogen

	1	2	3	4	5	6
1	7	1	0	0	0	2
2	1	6	2	0	0	0
3	0	2	6	1	0	0
4	0	0	1	7	2	0
5	0	0	0	2	6	1
6	2	0	0	0	1	6

Isomorphic is same in adjacent matrix (Isomers)

	1	2	3	4	5	6
1	7	2	0	0	0	1
2	2	6	1	0	0	0
3	0	1	6	2	0	0
4	0	0	2	7	1	0
5	0	0	0	1	6	2
6	1	0	0	0	2	6

The above matrices define the various kindly of domination atom connectivity and connectivity matrices with respect to the benezene compound.

Table 1 Different Engeries of Benzene molecule

Energy of Compound with hydrogen		
From Adjacency Matrix	From Atom Connectivity Matrix	From Connectivity Matrix
Energy = 14.6008	Energy = 17.7944 Isomer Energy = 17.7944	Energy = 42.0002 Isomer Energy = 42.0002
Energy of Compound without hydrogen		
From Adjacency Matrix	From Atom Connectivity Matrix	From Connectivity Matrix
Energy = 8	Energy = 12.9284 Isomer Energy = 12.9284	Energy = 36 Isomer Energy = 36
Domination Energy of Compound with hydrogen		
From Adjacency Matrix	From Atom Connectivity Matrix	From Connectivity Matrix
Energy = 14.941 (other dominating sets too)	Energy = 18.0398 Isomer Energy and other dominating sets too	Energy = 44.0001 Isomer Energy and other dominating sets too
Domination Energy of Compound without hydrogen		
From Adjacency Matrix	From Atom Connectivity Matrix	From Connectivity Matrix
Energy = 8.2926 (other dominating sets too)	Energy = 10.2857 Isomer Energy and other dominating sets too	Energy = 38.0001 Isomer Energy and other dominating sets too

There are various kinds of energies in the literature. Hence the above concept of atom connectivity and connectivity matrix will be applicable to all other kinds of energies defined in the literature. The different kinds of energies are found for few hydro carbons with different bond structure are listed and compared below.

The definition of the below energies with respect to atom connectivity and connectivity matrix can be referred in [24,25].

The energies of few simple hydro carbons are found and listed below. While comparing the various energies given below its found that in general ordinary energy less than atom connective energy less than connectivity energy. With few exceptions in Laplace energy as show below in the table 2, 3 and 4.

The main aim of this research is to relate the energy obtained from the compound to their physical properties. The question is still open to find the energy of compound is related to which physical property of the compound. Obtaining the physical property of the compound related to the energy will be considered a breakthrough in the field of chemistry and graph energies.

Table 2 Different Engeries of Ethyne

	Ethyne - C2H2					
	With hydrogen			Without hydrogen		
	Adj	ACM	CM	Adj	ACM	CM
Energy	4.5	7.2	14	2	6	12
Distance Energy	10.3	15.1	18	2	8	12
Laplace Energy	6	8.8	9.5	2	6	10
Laplace Distance Energy	13.7	18	14	2	8	10
Signless Laplace Energy	6	8.8	20	2	6	14
Signless Laplace Distance Energy	10.6	14	22	2	8	14
Laplacian Energy	4.8	7.5	14	2	6	12
Laplacian Distance Energy	10.7	15	17	2	8	12
Signless Laplacian Energy	4.8	7.5	14	2	6	12
Signless Laplacian Distance Energy	10.1	15.2	19	2	8	12
Domination Energy	4.8	7.3	16	2.2	6.1	13
Distance Domination Energy	9.7	14.2	20	2.2	8.1	13
Laplace Domination Energy	5.2	8.6	11.1	2.2	6.1	11
Laplace Distance Domination Energy	12.3	17.1	16	2.2	8.1	11

Signless Laplace Domination Energy	8	9.2	22	3	6.1	15
Signless Distance Laplace Domination Energy	12.5	14	24	3	8.1	15
Laplacian Domination Energy	4.5	7.6	16	2.2	6.1	13
Laplacian Distance Domination Energy	9.3	14.1	19	2.2	8.1	13
Signless Laplacian Domination Energy	5.8	7.6	16	2.2	6.1	13
Signless Laplacian Distance Domination Energy	10.5	14.5	21	2.2	8.1	13

Table 3 Different Engeries of Ethene

	Ethene - C2H4					
	With hydrogen			Without hydrogen		
	Adj	ACM	CM	Adj	ACM	CM
Energy	6	6.9	16	2	4	12
Distance Energy	20	23.4	26	2	6	122
Laplace Energy	10	10.8	8.7	2	4	10
Laplace Distance Energy	27.4	30.3	22	2	6	10
Signless Laplace Energy	10	10.8	26	2	4	14
Signless Laplace Distance Energy	20.7	20	30	2	6	14
Laplacian Energy	8.5	9.1	16	2	4	12
Laplacian Distance Energy	20.7	23.6	22	2	6	12
Signless Laplacian Energy	8.5	9.1	16.1	2	4	12
Signless Laplacian Distance Energy	20.9	23.4	30	2	6	12
Domination Energy	6.3	7.1	18	2.2	4.1	13
Distance Domination Energy	19.3	22	28	2.2	6.1	13
Laplace Domination Energy	8.8	10	10	2.2	4.1	11
Laplace Distance Domination Energy	25.7	28.8	24	2.2	6.1	11
Signless Laplace Domination Energy	12	12	28	3	4.1	15
Signless Distance Laplace Domination Energy	22.6	22	32	3	6.1	15
Laplacian Domination Energy	7.6	8.5	18	2.2	4.1	13
Laplacian Distance Domination Energy	19	22.1	24	2.2	6.1	13
Signless Laplacian Domination Energy	9.7	10.1	18	2.2	4.1	13
Signless Laplacian Distance Domination Energy	22.6	23.3	32	2.2	6.1	13

Table 4 Different Engeries of Ethane

	Ethane - C2H6					
	With hydrogen			Without hydrogen		
	Adj	ACM	CM	Adj	ACM	CM
Energy	7.2	7.2	18	2	2	12
Distance Energy	29.9	32.7	34	2	4	12
Laplace Energy	14	14	8.1	2	2	10
Laplace Distance Energy	41.2	43.7	30	2	4	10

Signless Laplace Energy	14	14	32	2	2	14
Signless Laplace Distance Energy	30.5	30	38	2	4	14
Laplacian Energy	12.3	12.3	18	2	2	12
Laplacian Distance Energy	30.7	33.2	26.5	2	4	12
Signless Laplacian Energy	12.3	12.3	18.5	2	2	12
Signless Laplacian Distance Energy	34.3	33.5	41.5	2	4	12
Domination Energy	7.5	7.5	20	2.2	2.2	13
Distance Domination Energy	29.2	31.1	36	2.2	4.1	13
Laplace Domination Energy	12.6	12.6	9.3	2.2	2.2	11
Laplace Distance Domination Energy	39.4	42	32	2.2	4.1	11
Signless Laplace Domination Energy	16	16	34	3	3	15
Signless Distance Laplace Domination Energy	32.7	32	40	3	4.1	15
Laplacian Domination Energy	11.2	11.2	20	2.2	2.2	13
Laplacian Distance Domination Energy	28.9	31.5	28.5	2.2	4.1	13
Signless Laplacian Domination Energy	13.7	13.7	20.3	2.2	2.2	13
Signless Laplacian Distance Domination Energy	36.2	35.5	43.5	2.2	4.1	13

5. FUTURE WORK

1. Find the various energies of different types of molecules.
2. Creating a database of all kind of energies for different types molecule.
3. Investigate the above energies with the properties of the molecules.
4. Investigate the relation between the various energies to the structural bonds of the molecule.
5. Investigate the relation between the various energies to the atoms present in the molecule.

6. DISCUSSION AND CONCLUSION

The potential advantages of this finding are that new techniques can be designed to obtain the energy of graphs, in which the specific property of the molecule can be obtained. This is of great importance in chemistry where the search for procedures to find the molecular properties is a golden rule for understanding such properties in structural terms. Finally, we hope that the new findings reported here would allow the researchers to understanding properties of the graph energy in molecules.

The energy of the graph has application with respect to the physical properties of the molecule. The above new and innovative approach of finding the energy of a specific compound gives a chance of the researchers to obtain the specific physical property of the compound which could be generalized for all compounds. The significant of the above energies is still open.

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