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Electronic and Optical Properties of Nanostructures and Its Relationship with Harari Index

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Abstract

The topological index of molecular graph is a number that attributed to the molecular graph and is valid than graph isomorphism, this number can reflect the properties of the molecules. In this study, Harari index in family phenacenes was calculated with some electronic and optical properties desired for a number of elements of the family, a model for predicting the electronic and optical properties by Harari index was prepared. To offer this model using mathematical software, electronic and optical properties of phenacenes calculated and compared with the data sources.

Keywords

Nanostructures, Harari Index, Electronic and Optical Properties, Gap Energy, Phenacenes

1. Introduction

Around mid-century theoretical chemists and physicists noted that various features of molecular structure of organic matter can be established by examining the appropriate structure to obtain the molecular graph. These graph constants are appropriate for the purposes of the physical and chemical and called topological indices. Topological indices are real numbers in terms of graph parameters (such as the degree of vertices, distances, etc.) in the study on molecular graphs presented in chemistry and physical and chemical properties of molecules can describe [1]. One of these topological indices, Harari index was introduced in 1991 by Professor Harari [2].

Today, scientists are trying to design and provide nanoscale electronic components. Manufacture nanoscale faced with limitations in many cases virtually impossible, therefore, due to small parts in recent years has led to

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the creation of nanostructures branch in electronics [3] [4].

Molecular electronic also called moltronic is a branch of nano-electronics that study the use of small groups of molecules in nano dimensions. Phenacenes are organic molecules that are highly regarded in molecular electronics and nanoscale. Because of the important electronic properties of the family, many research and studies have been done on them [5]. But in the molecules that the number of rings is more than six rings, measuring the electronic and optical properties needed to spend a long time and high cost. In these circumstances, there is a model for predicting the electronic and optical properties will be particularly important [6].

Definitions

Graph in mathematic is non-empty set of objects called vertices (V) are the vertices by lines called edges (E) connected and it show as $G = G(V, E)$. A molecular graph is simple graph, which is mainly composed of atoms of one molecule and the bonds between the atoms, are graph edges. In chemical graphs hydrogen atoms have been removed and will be ignored and the degree of each vertex is maximum 4 and all bonds between atoms are considered single.

Topological indexes are defined on the basis of graph theory [7] [8].

One of these topological indices, Harari index is defined by:

$$H = \left(\frac{1}{2}\right)\sum_{i=j}^{N}\sum_{j\neq i}^{N} d_{ij}^{-1} \tag{1}$$

where d_{ij} is elements of the distance matrix.

2. Methodology

The purpose of this paper is to obtain a simple model based on graph theory to predict optical and electronic properties of phenacenes.

Chemical formula phenacenes family is $C_{4n+2}H_{2n+4}$ with the $n \geq 2$. For example, the Harari index for $C_{10}H_8$ molecules is calculated. In **Figure 1**. The simple graph of the molecule is drawn.

According to **Figure 1**, the inverse matrix of $C_{10}H_8$ calculated in **Table 1**. Is as follows:

Using the Equation (1) Harari index for molecules $C_{10}H_8$ number 23.9 obtained (H = 23.9).

Harary index molecules $C_{4n+2}H_{2n+4}$ to n = 7 as well as the calculated and results in **Table 2** shown.

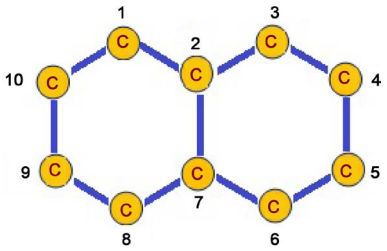

Figure 1. The simple graph of the molecule $C_{10}H_8$.

Table 1. The inverse matrix of $C_{10}H_8$.

$$d = \begin{pmatrix} 0 & 1 & 0.5 & 0.33 & 0.25 & 0.33 & 0.5 & 0.33 & 0.5 & 1 \\ 1 & 0 & 1 & 0.5 & 0.33 & 0.5 & 1 & 0.5 & 0.33 & 0.5 \\ 0.5 & 1 & 0 & 1 & 0.5 & 0.33 & 0.5 & 0.33 & 0.25 & 0.33 \\ 0.33 & 0.5 & 1 & 0 & 1 & 0.5 & 0.33 & 0.25 & 0.2 & 0.25 \\ 0.25 & 0.33 & 0.5 & 1 & 0 & 1 & 0.5 & 0.33 & 0.25 & 0.2 \\ 0.33 & 0.5 & 0.33 & 0.5 & 1 & 0 & 1 & 0.5 & 0.33 & 0.25 \\ 0.5 & 1 & 0.5 & 0.33 & 0.5 & 1 & 0 & 1 & 0.5 & 0.33 \\ 0.33 & 0.5 & 0.33 & 0.25 & 0.33 & 0.5 & 1 & 0 & 1 & 0.5 \\ 0.5 & 0.33 & 0.25 & 0.2 & 0.25 & 0.33 & 0.5 & 1 & 0 & 1 \\ 1 & 0.5 & 0.33 & 0.25 & 0.2 & 0.25 & 0.33 & 0.5 & 1 & 0 \end{pmatrix}$$

Table 2. Harary index molecules $C_{4n+2}H_{2n+4}$ to n = 7.

Chemical Formula	Simple Graph	IUPAC Name	H
$C_{10}H_8$		Naphthalene	23.9
$C_{14}H_{10}$		Phenanthrene	41.1
$C_{18}H_{12}$		Chrysene	60.7
$C_{22}H_{14}$		Picene	82.1
$C_{26}H_{16}$		Fulminene	104.9
$C_{30}H_{18}$		7-phenacene	129

3. Results

Some electronic and physical properties of phenacenes family ($C_{4n+2}H_{2n+4}$), the Ionization Energy, Bind Energy, Gap Energy and Electron Affinity Energy using software (Gaussian 09) was calculated and experimental data in the valid literature was compared. The results in **Table 3**. Had shown [6] [9] [10].

Using **Table 2** and **Table 3** data changes plot E_{gap} and E_{bind} in Harari index (H) in the **Figure 2** and **Figure 3** is drawn:

As the **Figure 2** and **Figure 3** can be predicted E_{gap} and E_{bind} in phenacenes family by the Harari index is possible and this prediction is very accurate, so that E_{bind} and E_{gap} carefully before $R^2 = 1$ predicted.

Figure 2 and **Figure 3** can be expected to provide the following relationships:

$$E_{gap} = 5\times10^{-9}H^5 - 2\times10^{-6}H^4 + 0.0003H^3 - 0.018H^2 + 0.5209H - 0.9661 \quad (2)$$

$$E_{bind} = 2\times10^{-9}H^5 - 7\times10^{-7}H^4 + 1\times10^{-4}H^3 - 0.0065H^2 + 0.1776H + 2.221 \quad (3)$$

Also in the Figures **Figure 4** and **Figure 5** changes diagram in both property Ionization Energy and Electron Affinity Energy of phenacenes family in term of Harari index (H) plotted.

Prediction of $E_{Ionization}$, $E_{Affinity}$ by the Harari index Figures **Figure 4** and **Figure 5** is associated with very high accuracy, so that predicted $E_{Ionization}$ and $E_{Affinity}$ will carefully $R^2 = 1$ is possible in the family phenacenes. The Ionization Energy ($E_{Ionization}$) and Electron Affinity Energy ($E_{Affinity}$) $C_{4n+2}H_{2n+4}$ molecules can be predicted by the following relationship:

$$E_{Affinity} = -2\times10^{-9}H^5 + 9\times10^{-7}H^4 - 0.0001H^3 + 0.0084H^2 - 0.2348H + 2.0301 \quad (4)$$

$$E_{Ionization} = 2\times10^{-9}H^5 - 8\times10^{-7}H^4 + 0.0001H^3 - 0.0073H^2 + 0.1957H + 5.9807 \quad (5)$$

4. Conclusions

As **Figures 2-5** shown using the Harari topological index, some electronic and optical properties of phenacenes family are given by $C_{4n+2}H_{2n+4}$ predict with great accuracy.

The success of the predicted energy gap E_{gap}, bind energy E_{bind}, ionization energy $E_{Ionization}$ and affinity electron energy $E_{Affinity}$ with Relations (2)-(5) is possible.

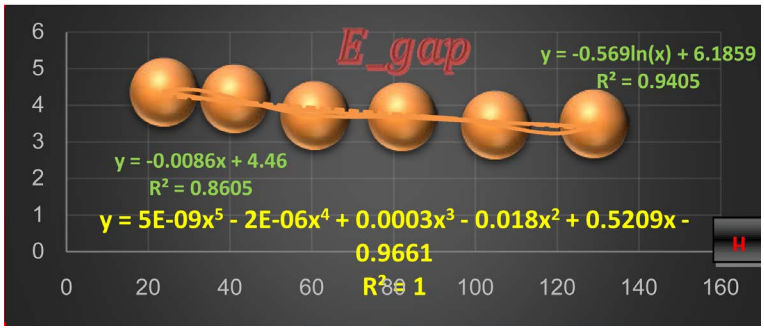

Figure 2. Changes plot E_{gap} in Harari index (H) for phenacenes family.

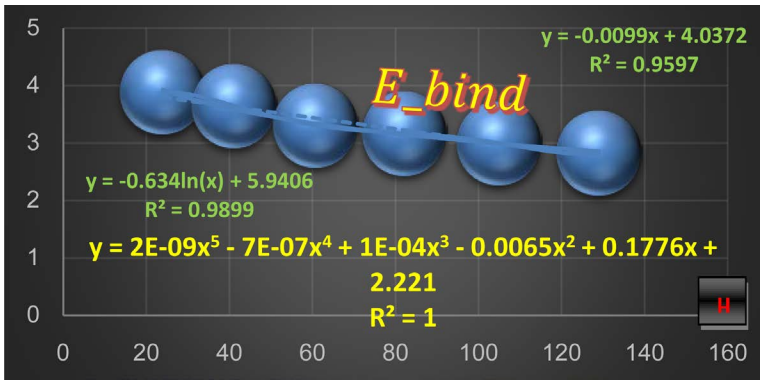

Figure 3. Changes plot E_{bind} in Harari index (H) for phenacenes family.

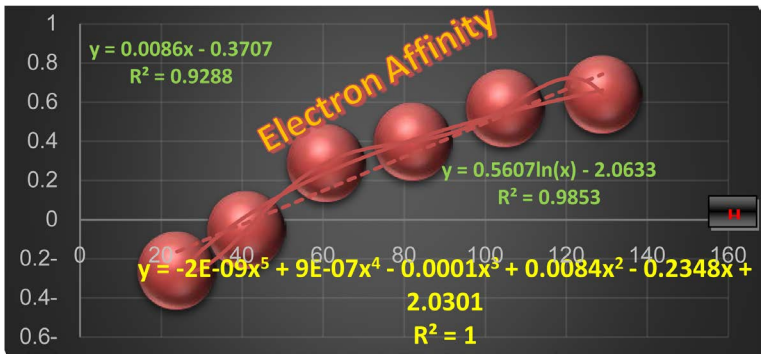

Figure 4. Changes plot $E_{Affinity}$ in Harari index (H) for $C_{4n+2}H_{2n+4}$.

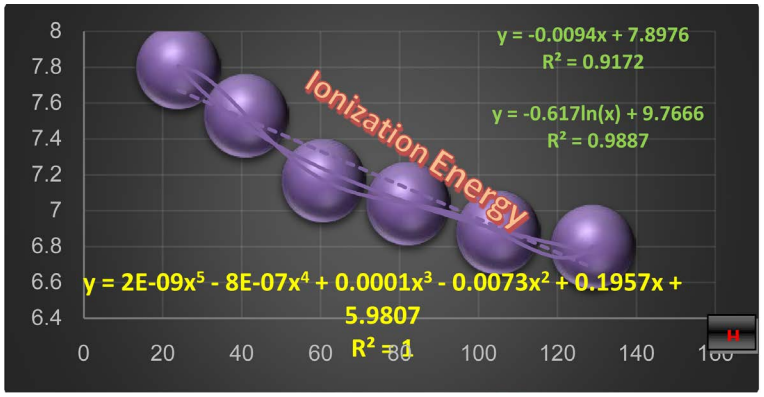

Figure 5. Changes plot $E_{Ionization}$ in Harari index (H) for $C_{4n+2}H_{2n+4}$.

Table 3. $E_{Affinity}$, E_{Gap}, $E_{Ionization}$ and E_{Bind} of phenacenes family.

Chemical Formula	IUPAC Name	E_{Bind} (ev)	$E_{Ionization}$ (ev)	E_{Gap} (ev)	$E_{Affinity}$ (ev)
$C_{10}H_8$	Naphthalene	3.89	7.8	4.36	−0.26
$C_{14}H_{10}$	Phenanthrene	3.65	7.53	4.19	−0.05
$C_{18}H_{12}$	Chrysene	3.31	7.17	3.73	0.29
$C_{22}H_{14}$	Picene	3.17	7.04	3.70	0.40
$C_{26}H_{16}$	Fulminene	3	6.88	3.47	0.57
$C_{30}H_{18}$	7-phenacene	2.83	6.80	3.50	0.64

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