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**RESEARCH ARTICLE**

# Some Electronic and Optical Properties of Nanostructures Using the First Zagreb Index

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## *Abstract*

Topological index of a molecular graph is a number that is attributed to molecular graph. This number can express some of the properties of molecules. In this article, the first Zagreb index was calculated in the family phenacenes and a suitable model was provided to predict the electronic and optical properties through first Zagreb index while considering some of the electronic and optical properties of a number of optional elements of this family. In order to propose this model, the electronic and optical properties of phenacenes were calculated by the computing software and then compared with the data in valid references.



## INTRODUCTION

Topological indices are real numbers that are presented as graph parameters (e.g., the degree of vertices, distances, etc.) during studies conducted on the molecular graphs in chemistry and can describe some physical and chemical properties of molecules [1]. The first Zagreb index is one of the topological indices, which was introduced by Professor Gutman(1972) [2].

Today, scientists are trying to design and provide electronic components in nanoscale. Manufacturing the nanoscale components has faced some limitations, which is virtually impossible in many cases. Thus, the attention paid to the nanostructures components in recent years has led to the emergence of nanostructures branch in electronics [3, 4].

Phenacenes are organic molecules that have received considerable attention in molecular electronics and nanoscale. Due to the important electronic properties of the family, many studies have been conducted on them [5]. However, in molecules with more than six rings, measuring electronic and optical properties is costly and time-consuming. In these circumstances, the existence of a suitable model to predict the electronic and optical properties is of special importance [6].

## Definitions

Mathematically, graph is a non-empty set of objects called vertices (V). The vertices are connected together by lines called edges (E) that are shown by G = G (V, E). A molecular graph is a simple graph whose vertex is mainly made up of atoms in a molecule and the bonds between atoms are the graph edges. In chemical graphs, hydrogen atoms were removed and excluded. Moreover, the degree of each vertex is a maximum of 4 and all bonds between atoms are considered as single. Topological indices are defined based on graph theory [7,8].

The first Zagreb index is one of the topological indices, which is defined as follows:

$$M_1(G) = \sum_{u \in V(G)} d^2(u) \qquad (1)$$

Where u is a member of the graph vertices and d is its degree [9, 10 and 11].

## Methods

This paper aims to obtain a simple model based on graph theory to predict the optical and electronic properties of phenacenes. Therefore, we first calculated the first Zagreb index for the family.
Chemical formula of the family phenacenes is $C_{4n+2}H_{2n+4}$ where $n \geq 3$.
Theorem:
If p and q are as the number of degrees 2 and 3 in the family of phenacenes :

$$M_1(G) = p(2)^2 + q(3)^2 \quad (2)$$

Then:

$$M_1(G) = 26n - 2 \quad (3)$$

Where n is number of rings.
Proof:
If N is graph vertices of phenacenes, thus:

$$P = (N/2) + 3 \quad (4)$$

$$q = (N/2) - 3 \quad (5)$$

Therefore:

$$M_1(G) = 4[(N/2) + 3] + 9[(N/2) - 3] \quad (6)$$

Since:

$$N = 4n + 2 \quad (7)$$

Equation (3) is proved.

## Calculation

For example, $M_1(G)$ was calculated for the molecule $C_{30}H_{18}$. Fig (1) plots the graph of this molecule.

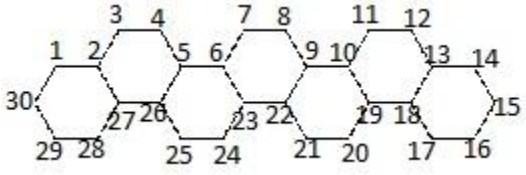


Fig (1): The graph of molecule $C_{30}H_{18}$

The first Zagreb index is equal to180 that is given in equation (3) for $C_{30}H_{18}$ molecule.
Tab (1) presents the first Zagreb index calculated for the family phenacenes.

Tab (1): The first Zagreb mass index of the family phenacenes ($C_{4n+2}H_{2n+4}$).

| IUPAC Name | $M_1(G)$ |
|---|---|
| phenanthrene | 76 |
| chrysene | 102 |
| picene | 128 |
| fulminene | 154 |
| 7-phenacene | 180 |

Electronic and physical properties of the phenacenes family ($C_{4n+2}H_{2n+4}$), namely, ionization energy, binding energy, gap energy, and electron affinity energy were calculated using Gaussian 09 software and the experimental data of references were compared with those mentioned in valid papers. Tab (2) shows the results [5, 12 and 13]:

Tab (2): Ionization Energy, Binding Energy, Gap Energy and the Electron Affinity Energy of the phenacenes family ($C_{4n+2}H_{2n+4}$) .

| **Chemical Formula** | **IUPAC Name** | **Electron Affinity(ev)** | **$E_{gap}$ (ev)** | **Ionization Energy(ev)** | **$E_{bind}$ (ev)** |
|---|---|---|---|---|---|
| $C_{10}H_8$ | phenanthrene | -0.05 | 4.19 | 7.53 | 3.65 |
| $C_{14}H_{10}$ | chysene | 0.29 | 3.73 | 7.17 | 3.31 |
| $C_{18}H_{12}$ | picene | 0.40 | 3.70 | 7.04 | 3.17 |
| $C_{22}H_{14}$ | fulminene | 0.57 | 3.47 | 6.88 | 3 |
| $C_{26}H_{16}$ | 7-phenacene | 0.64 | 3.50 | 6.80 | 2.83 |

## Results

Figs (2, 3) show the graph of changes in $E_{gap}$ and $E_{bind}$ according to the first Zagreb index ($M_1$).

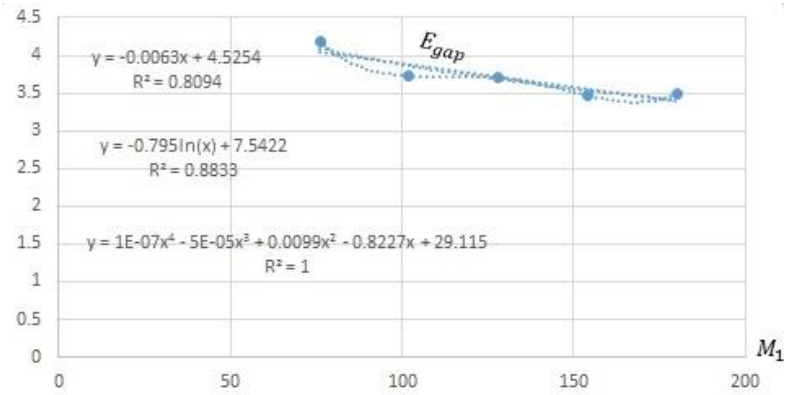


Fig (2): graph of changes in $E_{gap}$ according to the first Zagreb index ($M_1$).

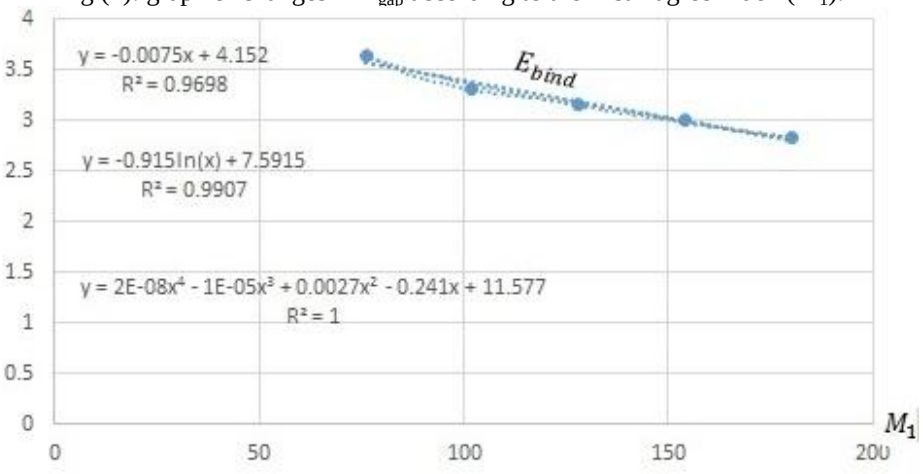


Fig (3): graph of changes in $E_{bind}$ according to the first Zagreb index ($M_1$).

As seen in Figs (2, 3) prediction of $E_{gap}$ and $E_{bind}$ in the family phenacenes might be made by the first Zagreb index. However, the prediction made by the index (Figs 2, 3) is much more accurate so that it well predicted $E_{bind}$ and $E_{gap}$ with $R^2$=1. These figures show the relations for prediction:

$$Egap = (1 \times 10^{-7})M_1{}^4 - (5 \times 10^{-5})M_1{}^3 + 0.0099M_1{}^2 - 0.8227M_1 + 29.115 \quad (8)$$

$$E_{bind} = (2 \times 10^{-8})M_1{}^4 - (1 \times 10^{-5})M_1{}^3 + 0.0027M_1{}^2 - 0.241M_1 + 11.577 \quad (9)$$

Moreover, Figs (4, 5) show the changes in both properties of ionization energy and electron affinity energy of phenacenes family according to the first Zagreb index ($M_1$), respectively.

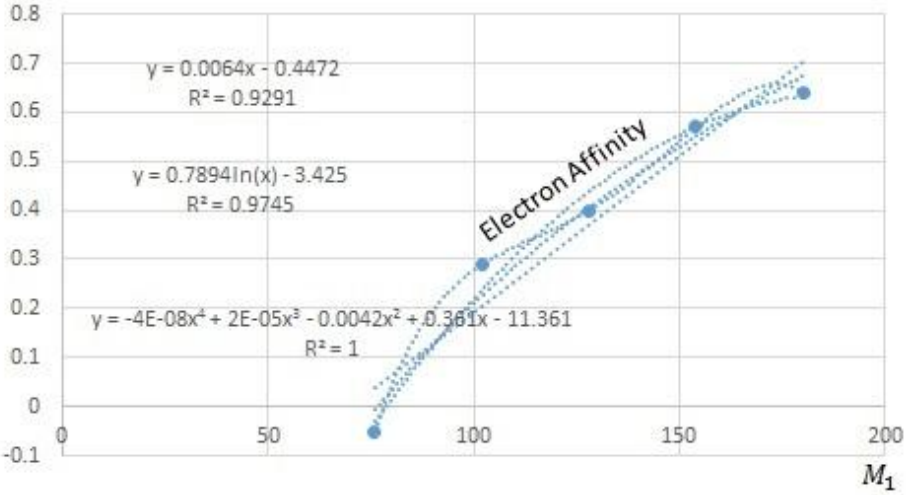


Fig (4): changes electron affinity ($E_{affinity}$) of the phenacenes according to the first Zagreb index ($M_1$).

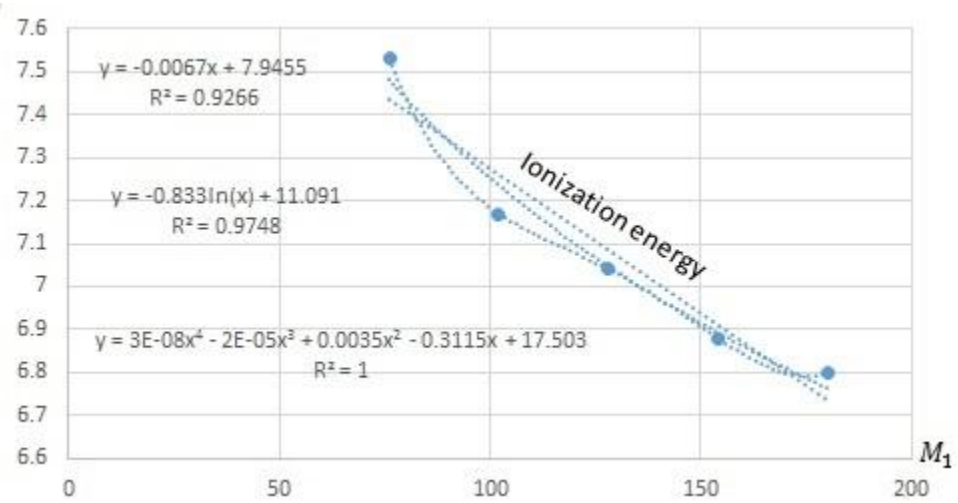


Fig (5): changes ionization energy ($E_{ionization}$) of the phenacenes according to the first Zagreb index ($M_1$).

The prediction of electron affinity energy and ionization energy brought about a very high accuracy through Zagreb index, with $R^2$=1(Figs 4, 5). Therefore, ionization energy ($E_{ionization}$) and electron affinity energy ($E_{affinity}$) of molecules $C_{4n+2}H_{2n+4}$ could be well predicted by the following relations:

$$E_{affinity} = -(4\times10^{-8})M_1{}^4 + (2\times10^{-5})M_1{}^3 - 0.0042M_1{}^2 + 0.361M_1 - 11.3611 \quad (10)$$

$$E_{ionization} = (3\times10^{-8})M_1{}^4 - (2\times10^{-5})M_1{}^3 + 0.0035M_1{}^2 - 0.3115M_1 + 17.503 \quad (11)$$

## Conclusion

As seen in Figs (4, 3, 4 and 5), some of the electronic and optical properties of phenacenes family, which is given by the molecule $C_{4n+2}H_{2n+4}$, could be carefully predicted by first Zagreb topological index. The success in predicting gap energy ($E_{gap}$), binding energy ($E_{bind}$), ionization energy ($E_{ionization}$), and electron affinity energy ($E_{affinity}$) is very noticeable that are given by relations (8 to 11).

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