



ISSN NO. 2320-5407

Journal homepage: <http://www.journalijar.com>

INTERNATIONAL JOURNAL
OF ADVANCED RESEARCH

RESEARCH ARTICLE

Prediction Electronic and Physical Properties of Nano Structures; Topological Index Method

Khakpoor; Ali Asghar

Department of Physics, Islamic Azad University- Central Tehran Branch, (IAUCTB)

Manuscript Info

Manuscript History:

Received: 14 April 2015
Final Accepted: 22 May 2015
Published Online: June 2015

Key words:

Ionization Energy; Electron Affinity Energy; Linear Acenes; Multiplicative First Zagreb Index; Topological Indices Method

*Corresponding Author

Khakpoor; Ali Asghar

Abstract

The production of electronic components on Nano scale is almost impossible due to various limitations and restrictions. Therefore, the scientists' attention to small pieces on natural scale in recent years resulted in the emergence of Nano-structures in electronic. Linear Acenes, with the chemical formula of $C_{4n+2}H_{2n+4}$, are a family of Organic Molecules which have absorbed attention in electronic Molecules and Nano scale. However, examining their electronic and optic features, especially when the number of rings is more than 6, is extremely costly and expensive. This study aims at presenting a model to predict electro-optic features of Linear Acenes through Topologic Index Method. The Topologic Index of a Molecular graph is a number which describes molecule characteristics. Multiplicative First Zagreb Index is one of the Topologic Indices which was examined and measured in Linear Acenes Family. Then, through measuring Ionization Energy and Electron Affinity Energy for some members of the family and comparing them with the findings of authentic researches, we were able to present an affective model for predicting electronic and optic features of Acenes.

Copy Right, IJAR, 2015,. All rights reserved

INTRODUCTION

Nowadays, the scientists attempt to design and produce Nano metric electronic components. The production of electronic components on Nano scale is almost impossible due to various limitations and restrictions. Therefore, the scientists' attention to small pieces on natural scale in recent years resulted in the emergence of Nano-structures in electronic [1], [2]. Acenes, with the chemical formula of $C_{4n+2}H_{2n+4}$, are a family of Organic Molecules which have absorbed attention in electronic Molecules and Nano scale. Based on the findings, large Acenes, with six to ten rings, are found in volcano ash and interplanetary dust and are very suitable for electronic components [3]. This group of elements has been studied for its important electronic features; however, examining their electro-optic features, if they have more than six rings, is extremely costly and expensive [4].

Topologic Indexes are Real Numbers which were introduced during chemistry studies on molecular graphs and are presented according to graph parameters such as outline level and the distance between vertices. Describing and predicting chemical, physical, and electronical features of the molecule is possible [5], [6], [7]. One of these indices, is the Multiplicative First Zagreb Index, in 2011 by Professor Guttmann and his colleagues, was introduced [8].

A. Definitions

Graph is a set of occupied materials, called vertices, linked together with lines called Edge and shown as $G=(V, E)$. A molecular graph is a simple one whose vertices is made of single molecular atoms and graph Edges are actually the bonds between atoms. In chemical graphs, hydrogen is removed, the value each vertices is maximum 4

and all bonds between atoms are considered to be single [9], [10], [11]. Multiplicative First Zagreb Index is defined as the following [8], [12], [13]:

$$\Pi_1(G_1) = \prod_{u \in V(G)} (d_G(u))^2 \tag{1}$$

Where $d_G(u)$, is the degree of u vertex in graph G .

Methods

To get a simple model based on graph theory with the potential of predicting electronic and optic features in Linear Acenes, first we have to examine and measure Multiplicative First Zagreb Index in this family of elements. Therefore, the simple molecular graph of Linear Acenes family might be something like the Fig (1):

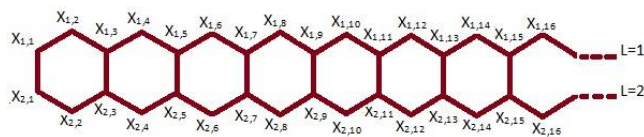


Fig (1): Simple molecular graph of Linear Acenes family

Theorem 1: suppose n represents the number of rings in Linear Acenes family; thus, $\Pi_1(G)$ index equals:

$$\Pi_1(G) = 4^{(2n+4)}9^{(2n-2)} \tag{2}$$

Argument: consider simple graph in Fig (1) which can be explained from two different perspectives:

I. All vertices and Edges located on and above surface $L=1$ are called G_1 , Fig (2):

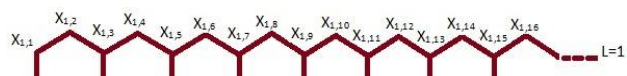


Fig (2): G_1 is all vertices and Edges located on and above surface $L=1$

II. All vertices and Edges located on and below surface $L=2$ are called G_2 , Fig (3):

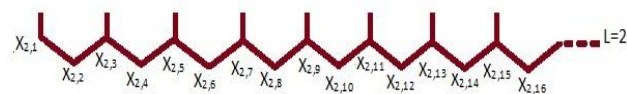


Fig (3): G_2 is all vertices and Edges located on and below surface $L=2$

In this case, Multiplicative First Zagreb index for relation 1 for G_1 is as the following:

$$\Pi_1(G_1) = \prod_{m=1}^k d_{1,m}^2 \tag{3}$$

If we separate first and last sentences in relation (3) which is related to $X_{1,1}$ and $X_{1,1}$ vertices, then we have:

$$\Pi_1(G_1) = d_{1,1}^2 d_{1,k}^2 \prod_{m=2}^{k-1} d_{1,m}^2 \tag{4}$$

Also, since $X_{1,m}$ value based on m being even and odd, are the same, relation (4) changes like this:

$$\Pi_1(G_1) = d_{1,1}^2 d_{1,k}^2 \left[\prod_{i=1}^{\frac{k-1}{2}} d_{1,2i}^2 \right] \left[\prod_{i=1}^{\frac{k-3}{2}} d_{1,2i+1}^2 \right] \tag{5}$$

$$\Pi_1(G_1) = 4^2 \left[4^{\binom{k-1}{2}} \right] \left[9^{\binom{k-3}{2}} \right] \tag{6}$$

Since $k = 2n + 1$, by putting it in relation (6) we have:

$$\Pi_1(G_1) = 4^{(n+2)}9^{(n-1)} \tag{7}$$

Based on Figs (2) and (3) and the similarity of G_1 and G_2 , we conclude that:

$$\Pi_1(G_2) = 4^{(n+2)}9^{(n-1)} \quad (8)$$

And then, relations (7) and (8) are used to prove the theorem.

$$\Pi_1(G) = [\Pi_1(G_1)][\Pi_1(G_2)] = 4^{(2n+4)}9^{(2n-2)} \quad (9)$$

Results

Based on relation 9, $\Pi_1(G)$ Index for the first five elements of the Linear Acenes family was measured and shown in table (1).

Table(1): $\Pi_1(G)$ Index in Linear Acenes Family.

IUPAC name	Chemical formula	$\Pi_1(G)$
naphthalene	C ₁₀ H ₈	(4) ⁸ (9) ²
anthracene	C ₁₄ H ₁₀	(4) ¹⁰ (9) ⁴
tetracene	C ₁₈ H ₁₂	(4) ¹² (9) ⁶
pentacene	C ₂₂ H ₁₄	(4) ¹⁴ (9) ⁸
hexacene	C ₂₆ H ₁₆	(4) ¹⁶ (9) ¹⁰

To examine electronic and optical properties, Ionization Energy and Electron Affinity Energy were calculated and compared according to authentic sources [14], [15]. Results are shown in table (2).

Table (2): Ionization Energy and Electron Affinity Energy for Linear Acenes.

Chemical formula	IUPAC name	E _{affinity} (ev)	E _{Ionization} (ev)
C ₁₀ H ₈	naphthalene	-0.26	7.80
C ₁₄ H ₁₀	anthracene	0.35	7.02
C ₁₈ H ₁₂	tetracene	1.08	6.49
C ₂₂ H ₁₄	pentacene	1.48	6.12
C ₂₆ H ₁₆	hexacene	1.78	5.83

Fig (4) shows Ionization Energy changes in Linear Acenes according to $\text{Ln}[\Pi_1(G)]$. This Figure shows the success and effectiveness of Multiplicative First Zagreb Index in predicting Ionization Energy in Linear Acenes. This accuracy is about $R^2=0.9979$ and is shown through relation (10)

$$E_{\text{ioniz.}} = -1.885 \text{Ln}[\text{Ln}[\Pi_1(G)]] + 12.931 \quad (10)$$

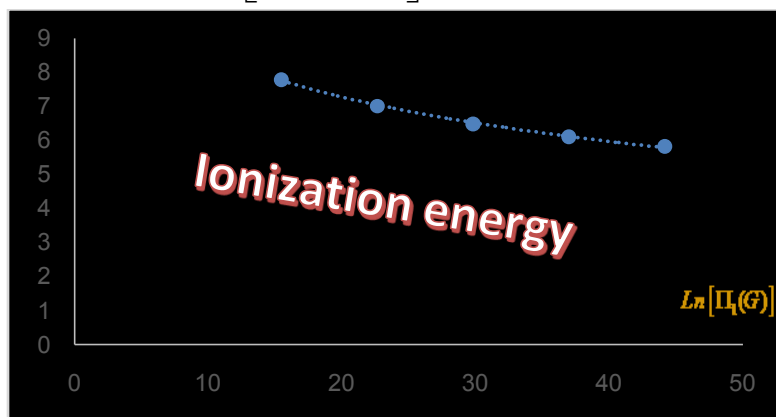


Fig (4): Ionization Energy changes in Linear Acenes according to $\text{Ln}[\Pi_1(G)]$.

Fig (5) shows Electron Affinity Energy changes in Linear Acenes according to $\text{Ln}[\Pi_1(G)]$.

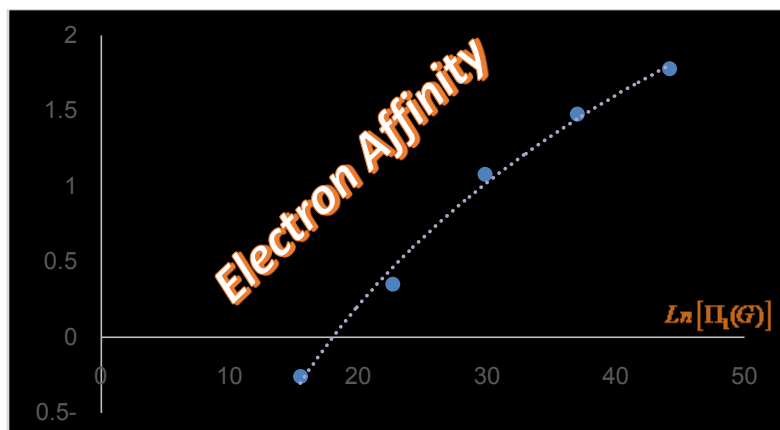


Fig (5): Electron Affinity Energy changes in Linear Acenes according to $Ln[\Pi_1(G)]$.

Fig (5) shows high accuracy level of Multiplicative First Zagreb Index in predicting Electron Affinity Energy of Linear Acenes with $R^2=0.9927$. This success is made possible with relation (11).

$$E_{Aff\ int\ y} = 2.0114Ln[Ln[\Pi_1(G)]] - 5.8135 \quad (11)$$

Conclusion

Using TIM predict some physical and electro-optical properties of nano structure materials possible. This is particularly important, when using experimental methods with a waste of time and financial cost is enormous, and theoretical methods have failed in fulfilling. In the Linear Acenes family with increasing of loops; the situation is more difficult, more complex and more expensive. Here, with the help of TIM method and relations (10) and (11), we have been able to predict Ionization Energy and Electron Affinity Energy in Linear Acenes. This prediction was done for five heavy elements of Linear Acenes through TIM method, and the results are shown in table (3).

Table (3): Prediction of Electron Affinity Energy, and Ionization Energy for 5- heavier member in Linear Acenes using TIM.

Chemical formula	$\Pi_1(G)$	$E_{affinity}$ (ev)	$E_{ionization}$ (ev)
$C_{30}H_{18}$	$(4^{18})(9^{12})$	2.1075	5.5077
$C_{34}H_{20}$	$(4^{20})(9^{14})$	2.3704	5.2613
$C_{38}H_{22}$	$(4^{22})(9^{16})$	2.7333	5.0434
$C_{42}H_{24}$	$(4^{24})(9^{18})$	2.8113	4.8481
$C_{46}H_{26}$	$(4^{26})(9^{20})$	3.0002	4.6711

Acknowledgments

I would like to thank Islamic Azad University Central Tehran Branch (IAUCTB) for helpful protections.

References

- [1]. P´erez-Jim´enez A. J. and Sancho-Garca J. C., J. Am. Chem. Soc. 131 (2009), 14857.
- [2]. Sancho-Garc´ia J. C., P´erez-Jim´enez A. J., Phys. Chem. Chem. Phys. 11 (2009), 2741.
- [3]. Jiang D., Dai S., Chem. Phys. Lett. 466, (2008), 72.
- [4]. Lias S., Ionization energy evaluation, in: P. J. Linstrom, W. G. Mallard (Eds.), NIST Chemistry WebBook, NIST Standard Reference Database Number 69, National Institute of Standards and Technology Gaithersburg MD, (2005).
- [5]. Bonchev D., Information theoretic for characterization of chemical structures, Reserch studies press,, Latchworth, (1983).
- [6]. Khakpoor A.A., Agahi Keshe B., IJAR, 3, 5, (2015), 548-551.
- [7]. Khakpoor A. A., Agahi Keshe B., IJCR 7, 5, (2015), 15686-15689.
- [8] Gutman I., Multiplicative Zagreb indices of trees, Bull. Soc. Math. Banja Luka, 18, (2011), 17–23.
- [9]. Bondy J. A., Murty U. S. R., Graph Theory with Applications, MacMillan, London, (1976).
- [10]. Trinajstic N., chemical Graph Theory, 2nd edition, CRC press, Boca Raton, FL, (1992).
- [11]. Ezra G.S., symmetry properties of Molecules,lecture Notes in chemistry 28,(Springer,Germany, (1982).

- [12]. Todeschini R., Ballabio D., Consonni V., Novel molecular descriptors based on functions of new vertex degrees, in: I. Gutman, B. Furtula (Eds.), *Novel Molecular Structure Descriptors — Theory and Applications I*, Univ. Kragujevac, Kragujevac, pp. 73–100, (2010).
- [13] Todeschini R., Consonni V., New local vertex invariants and molecular descriptors based on functions of the vertex degrees, *MATCH Commun. Math. Comput. Chem.* 64 (2010), 359–372.
- [14]. Kadantsev E. S., Stott M. J., Rubio A., *J. Chem. Phys.* 124 (2006), 134901.
- [15]. Mallocci G., Mulas G., Cappellini G., Joblin C., *Chem. Phys.* 340 (2007).