

# A Model for Computing Gap Energy and Electron Affinity Energy of Carbon Nanostructures

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**Abstract** Molecular electronic, which is supposed to replace silicon electronic in the future, is an incipient branch of Nanotechnology which focusing on the organic molecules. Since recognizing and examining this family of nano-structures needs long time and very expensive, an appropriate pattern to predict electronic properties is very beneficial; Topological Indices Method (TIM) is a useful approach for this purpose. Therefore, it is first tried to produce a relationship between the topological indices based on the number of rings; then the ISI index values are calculated for Circumacenes family. The gap energy and electron affinity energy of Circumacenes family ( $C_{8(n+2)/3}H_{(2n+22)/3}$ ) were calculated using Gaussian 09 software and compared to the validated results from experiments and other references. The opto-electronics properties of Circumacenes family were described by ISI index. Finally, some heavier members of Circumacenes family are exposed to TIM method to predict of energy gap, and electron affinity energy.

**Keywords** Molecular Electronic, Carbon Nanostructures, Circumacenes, Gap Energy, Electron Affinity

supposed to replace silicon electronic in the future, is an incipient branch of Nano-technology. Since minifying the size of electronic components on Nano-scale confronts various limitations, focusing on the molecular electronic is a considerable point which should attract attention. The molecular electronic is a branch of science based on Nano-technology with multiple applications in electronic industry in which organic molecules are central. Aromatic hydrocarbon from the root of benzene can provide suitable environments for electron transition due to p orbitals, upper and lower electron clouds, and resonance phenomenon. Electronic circuits and logic gates are designed out of the joining of these hydrocarbons [1-4].

Circumacenes is a family of organic molecules with the chemical formula of  $C_{8(n+2)/3}H_{(2n+22)/3}$  which is focused in molecular electronic [5-6]. Since recognizing and examining this family of Nano-structures needs huge time and money, an appropriate pattern to predict electronic features is very beneficial; Topological Indices Method (TIM), is a cheap and useful approach to gain this goal [7-13]. A single number, representing a chemical structure in graph-theoretical terms via the molecular graph, is called a topological descriptor and if it in addition correlates with a molecular property it is called topological index; it is used to understand physicochemical properties of chemical compounds. Topological indices are interesting since they capture some of the properties of a molecule in a single number. Hundreds of topological indices have been introduced and studied, starting with the work by Wiener in which he used the sum of all shortest-path distances of a (molecular) graph for modeling physical properties of alkanes [14].

## 1. Introduction

Today's knowledge requires increasing the capacity of data restoration, data transition, and making electronic components as small as possible; the electronic components' being smaller not only increases the speed of the process, but also reduces the amount of consumed energy, two important goals which are accessible through Nano-electronic technique. The electronic industry is based on silicon is 50 years old and has gradually matured technologically, industrially, and financially. Molecular electronic, which is

## 2. Materials and Methods

### 2.1. Definition

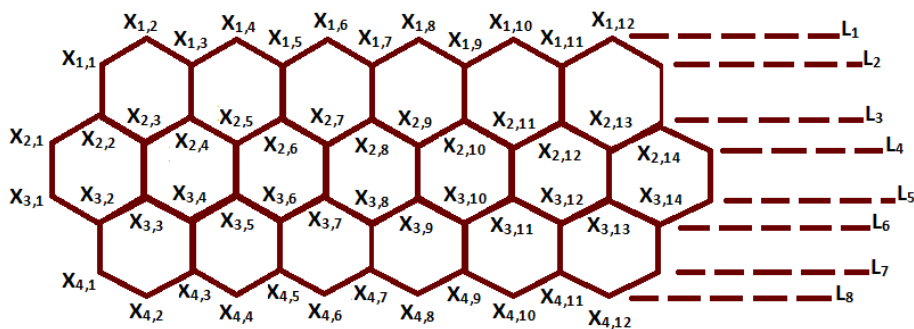


Figure 1. Simple molecular graph of Circumacenes ( $C_{(8n+16)/3}H_{(2n+22)/3}$ ).

In mathematical, a non-empty set of objects identified as vertices ( $V$ ) is called a graph. This vertices are connected by lines called edge ( $E$ ), and are showed as  $G = G(V, E)$ . A molecular graph is a simple graph whose vertices are composed from the atoms of a molecule, and bonds between atoms of the molecule make up edges of the graph. In chemical graphs hydrogen atoms are removed, and they are discarded. Dehydrogenized graph is said to these graphs in phrase. As well as all bonds between the atoms are considered as unique, and the degree of each vertex will be 4 maximally [15-16]. One of the topological indices is ISI index which is defined as (1) [17]:

$$ISI(G) = \sum_{uv \in E(G)} \frac{1}{\frac{1}{d_u} + \frac{1}{d_v}} = \sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v} \quad (1)$$

Where  $d_u$  and  $d_v$  are degrees of  $u$  and  $v$  vertices, respectively, and they have a common bond together.

## 2.2. Methods

It is first tried to produce a relationship between the topological indices based on the number of rings; then ISI index values are calculated for some members of Circumacenes family. Consider simple graph of Circumacenes family ( $C_{(8n+16)/3}H_{(2n+22)/3}$ ) as presented in Figure 1.

Theorem 1: Suppose  $n$  is the number of rings in Circumacenes family; therefore ISI index equals to:

$$ISI(G) = \frac{61n + 53}{15} \quad (2)$$

Proof: Imagine a simple molecular graph which can be explicated from nine areas:

- I. All vertices and edges that are located between  $L_1$  and  $L_2$  levels and it is called  $G_1$ .
- II. All vertices and edges that are located between  $L_2$  and  $L_3$  levels and it is called  $G_2$ .
- III. All vertices and edges that are located between  $L_3$  and  $L_4$  levels and it is called  $G_3$ .
- IV. All vertices and edges that are located between  $L_4$  and  $L_5$  levels and it is called  $G_4$ .
- V. All vertices and edges that are located between  $L_5$

- and  $L_6$  levels and it is called  $G_5$ .
- VI. All vertices and edges that are located between  $L_6$  and  $L_7$  levels and it is called  $G_6$ .
- VII. All vertices and edges that are located between  $L_7$  and  $L_8$  levels and it is called  $G_7$ .

For  $G_1$ , using (1), we have:

$$ISI(G_1) = \sum_{m=1}^{k-1} \frac{d_{1,m} d_{1,m+1}}{d_{1,m} + d_{1,m+1}} \quad (3)$$

The first and last terms are separated:

$$ISI(G_1) = \sum_{m=1}^{k-1} \frac{d_{1,m} d_{1,m+1}}{d_{1,m} + d_{1,m+1}} = \frac{d_{1,1} d_{1,2}}{d_{1,1} + d_{1,2}} + \frac{d_{1,k-1} d_{1,k}}{d_{1,k-1} + d_{1,k}} + \sum_{m=2}^{k-2} \frac{d_{1,m} d_{1,m+1}}{d_{1,m} + d_{1,m+1}} \quad (4)$$

And for the first two terms in (4) we have

$$\frac{d_{1,1} d_{1,2}}{d_{1,1} + d_{1,2}} = \frac{d_{1,k-1} d_{1,k}}{d_{1,k-1} + d_{1,k}} = 1 \quad (5)$$

And for  $m \neq 1$  and  $m \neq k$  we will have:

$$\frac{d_{1,m} d_{1,m+1}}{d_{1,m} + d_{1,m+1}} = \frac{6}{5} \quad (6)$$

And though (5) and (6), we can conclude:

$$ISI(G_1) = 1 + 1 + \sum_{m=2}^{k-2} \frac{6}{5} = 2 + \frac{6}{5}(k-3) \quad (7)$$

And since  $k = (2n+1)/3$ , therefore:

$$ISI(G_1) = 2 + \frac{6}{5} \left( \frac{2n-8}{3} \right) \quad (8)$$

In  $G_2$ , first we separate first and last terms:

$$ISI(G_2) = \sum_{m=1}^k \frac{d_{1,m} d_{2,m}}{d_{1,m} + d_{2,m}} = \frac{d_{1,1} d_{2,1}}{d_{1,1} + d_{2,1}} + \frac{d_{1,k} d_{2,k}}{d_{1,k} + d_{2,k}} + \sum_{m=2}^{k-1} \frac{d_{1,m} d_{2,m}}{d_{1,m} + d_{2,m}} \quad (9)$$

Equation (9) signifies for the first two terms as:

$$\frac{d_{1,1}d_{2,1}}{d_{1,1}+d_{2,1}} = \frac{d_{1,k}d_{2,k}}{d_{1,k}+d_{2,k}} = \frac{6}{5} \quad (10)$$

And for two terms of  $m \neq 1$  and  $m \neq k$ , we have:

$$\frac{d_{1,m}d_{2,m}}{d_{1,m}+d_{2,m}} = 1 \quad (11)$$

Equations (10) and (11) will lead to:

$$ISI(G_2) = \frac{6}{5} + \frac{6}{5} + \sum_{m=2}^{k-1} 1 = \frac{12}{5} + (k-2) \quad (12)$$

And since  $k = (n+2)/3$ , so:

$$ISI(G_2) = 2 + \frac{6}{5} \left( \frac{n-4}{3} \right) \quad (13)$$

In  $G_3$ , first we separate first and last terms:

$$ISI(G_3) = \sum_{m=1}^{k-1} \frac{d_{2,m}d_{2,m+1}}{d_{2,m}+d_{2,m+1}} = \frac{d_{2,1}d_{2,2}}{d_{2,1}+d_{2,2}} + \frac{d_{2,k-1}d_{2,k}}{d_{2,k-1}+d_{2,k}} + \sum_{m=2}^{k-2} \frac{d_{2,m}d_{2,m+1}}{d_{2,m}+d_{2,m+1}} \quad (14)$$

Equation (14) signifies for the first two terms as:

$$\frac{d_{2,1}d_{2,2}}{d_{2,1}+d_{2,2}} = \frac{d_{2,k-1}d_{2,k}}{d_{2,k-1}+d_{2,k}} = \frac{6}{5} \quad (15)$$

And for two terms of  $m \neq 1$  and  $m \neq k$ , we have:

$$\frac{d_{2,m}d_{2,m+1}}{d_{2,m}+d_{2,m+1}} = 1 \quad (16)$$

Equations (15) and (16) will lead to:

$$ISI(G_3) = \frac{6}{5} + \frac{6}{5} + \sum_{m=2}^{k-2} 1 = \frac{12}{5} + (k-3) \quad (17)$$

And since  $k = (2n+7)/3$ , so:

$$ISI(G_3) = \frac{12}{5} + \left( \frac{2n-2}{3} \right) \quad (18)$$

For  $G_4$ , we can write:

$$ISI(G_4) = \sum_{m=1}^k \frac{d_{2,m}d_{3,m}}{d_{2,m}+d_{3,m}} \quad (19)$$

The first and last terms are separated:

$$ISI(G_4) = \frac{d_{2,1}d_{3,1}}{d_{2,1}+d_{3,1}} + \frac{d_{2,k}d_{3,k}}{d_{2,k}+d_{3,k}} + \sum_{m=2}^{k-1} \frac{d_{2,m}d_{3,m}}{d_{2,m}+d_{3,m}} \quad (20)$$

And for the first two terms in (20), we have

$$\frac{d_{2,1}d_{3,1}}{d_{2,1}+d_{3,1}} = \frac{d_{2,k}d_{3,k}}{d_{2,k}+d_{3,k}} = 1 \quad (21)$$

And for  $m \neq 1$  and  $m \neq k$  we will have:

$$\frac{d_{2,m}d_{3,m}}{d_{2,m}+d_{3,m}} = 1 \quad (22)$$

And though (21) and (22), we can conclude:

$$ISI(G_4) = 1 + 1 + \sum_{m=2}^{k-1} 1 = 2 + (k-2) \quad (23)$$

And since  $k = (n+5)/3$ , therefore:

$$ISI(G_4) = 2 + \left( \frac{n-1}{3} \right) \quad (24)$$





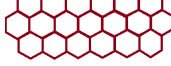
The calculation procedure of  $G_5$ ,  $G_6$  and  $G_7$  areas are the same as  $G_3$ ,  $G_2$  and  $G_1$  respectively and is given through (18), (10) and (13), Therefore,

$$ISI(G) = ISI(G_1) + ISI(G_2) + ISI(G_3) + ISI(G_4) + ISI(G_5) + ISI(G_6) + ISI(G_7) \quad (25)$$

So, (2) is achieved and theorem is proved.

Then ISI index is calculated for some Circumacenes family members using (2) and the results are shown in Table 1.

**Table 1.** ISI index for the first five members of Circumacenes family

Chemical Formula	IUPAC Name	Simple Graph	ISI Index
C <sub>24</sub> H <sub>12</sub>	coronene		32
C <sub>32</sub> H <sub>14</sub>	ovalene		44.2
C <sub>40</sub> H <sub>16</sub>	circumanthracene		56.4
C <sub>48</sub> H <sub>18</sub>	circumtetracene		68.6
C <sub>56</sub> H <sub>20</sub>	circumpentacene		80.8

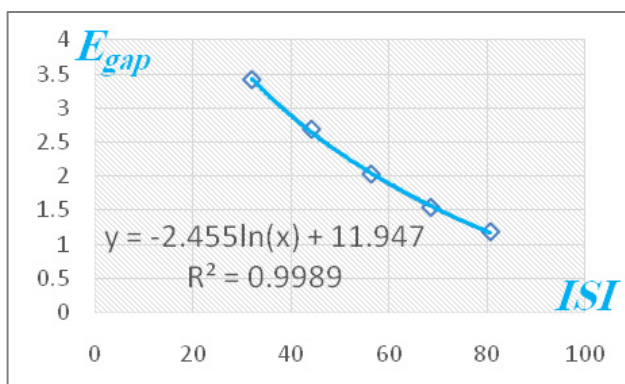
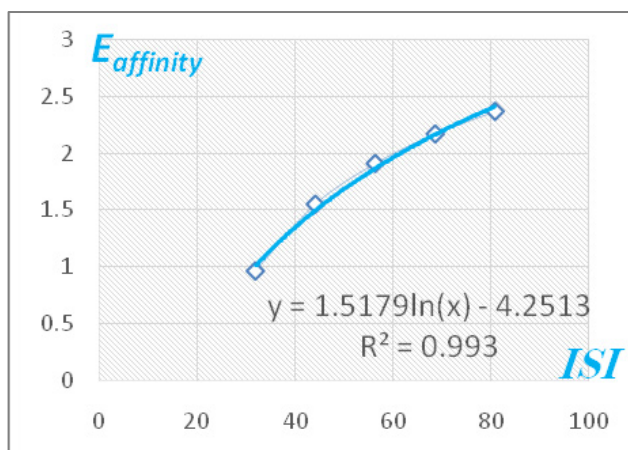
## 4. Results

Electro-optical properties of Circumacenes family (C<sub>8(n+2)/3</sub>H<sub>(2n+22)/3</sub>) including of gap energy and electron affinity energy, were calculated using Gaussian 09 software and compared to the validated results from experiments and other references as given in Table 2. [18-19].

**Table 2.** Energy gap and electron affinity energy of the first five members of Circumacenes family

Chemical Formula	$E_{\text{affinity}}$ (ev)	$E_{\text{gap}}$ (ev)
$C_{24}H_{12}$	0.96	3.42
$C_{32}H_{14}$	1.55	2.69
$C_{40}H_{16}$	1.91	2.03
$C_{48}H_{18}$	2.17	1.54
$C_{56}H_{20}$	2.37	1.18

Figures 2 and 3 respectively show gap energy changes and electron affinity energy changes for Circumacenes family according to ISI index as the results of this work.

**Figure 2.** Gap energy changes in Circumacenes family according to ISI index.**Figure 3.** Electron affinity energy changes in Circumacenes family according to ISI index.

As it is shown in Figure 2, the gap energy can be calculated via ISI index changes for Circumacenes family, with a high level of precision ( $R^2=0.9989$ ). This prediction is possible using (26).

$$E_g = -2.455 \ln(ESI) + 11.947 \quad (26)$$

This prediction has been performed with a precision of  $R^2=0.993$  for electron affinity energy, by (27).

$$E_{\text{affinity}} = 1.5179 \ln(ESI) - 4.2513 \quad (27)$$

## 5. Conclusions

Table 3 shows the calculation results of gap energy and electron affinity energy of Circumacenes family through the TIM method. Table 3 shows the validity of the TIM method in a comparison of results with the reference values (Table 2).

**Table 3.** Calculation of energy gap and electron affinity energy of Circumacenes family through the TIM method

Chemical Formula	$E_{\text{affinity}}$ (ev)	$E_{\text{gap}}$ (ev)
$C_{24}H_{12}$	1.0093	3.4386
$C_{32}H_{14}$	1.4996	2.6456
$C_{40}H_{16}$	1.8695	2.0472
$C_{48}H_{18}$	2.1668	1.5665
$C_{56}H_{20}$	2.4152	1.1646

As it is shown, prediction of some physical and electro-optic properties of Circumacenes family with high precision is possible through the TIM method and ISI index. The significance of this method is magnified in the case of heavier elements in article theoretical and experimental methods, wasting much time and money still giving approximated results. Hereafter, some heavier members of Circumacenes family are exposed to the TIM method. Equations 26 and 27 have been used to predict the energy gap and electron affinity energy. The results are shown in Table 4.

**Table 4.** Predicting energy gap and electron affinity energy through the TIM method

Chemical Formula	ISI Index	$E_{\text{Affinity}}$ (ev)	$E_{\text{Gap}}$ (ev)
$C_{64}H_{22}$	93	2.6287	0.8194
$C_{72}H_{24}$	105.2	2.8158	0.5168
$C_{80}H_{26}$	117.4	2.9823	0.2474
$C_{88}H_{28}$	129.6	3.1324	0.0047

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