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THE EFFECTS OF CYCLOEPENTANES ON ELECTRONIC AND SPECTRA PROPERTIES OF NANOTUBES MOLECULES

RAJAA K. MOHAMMAD[1,*], SHUROOQ SABAH ABED AL-ABBAS[2]

[1]Department of Physics, College of Science, University of Kerbala , Karbala, Iraq
[2]Department of Physics, College of Education for Pure Sciences, University of Babylon, Hilla, Iraq
*Corresponding Author: rajaa.k@uokerbala.edu.iq

Abstract

In this research, we examine the electronic structure and structural properties of nanotubes (CNT) (4,0) with the Cycloepentanes doped in the same sites. The structural and electronic properties that are investigated are energy bandgap, electron affinity, ionization potential, density of states (DOS), Fermi energy (E_f) and IR spectra. This doping result in decreasing the energy gap values with increasing the ionization potential, electron affinity, this, which make this CNTs under study have semiconductor behaviors. This doping also reduced the of HOMO and LUMO values, total energy and different the shape of the DOS. The CNT-Cyclopentadine has small energy gap is (1.245175) eV compared with all molecules under study. From this research all molecules are very important in many applications.

Keywords: Cycloepentanes, Electronic and spectra properties, Nanotubes molecules.

1. Introduction

Carbon nanotubes (CNTS) are hollowed cylinders made up of one or many graphite sheets that are quasi-one-dimensional crystals. Despite the fact that (CNTS) are made up of carbon atoms, its physical characteristics can differ greatly relying on the microscopic arrangement of tube. The noticeable feature is either metallic or semiconductor nature: about two-thirds (2/3) of the conceivable nanotube architectures are semiconducting and one-third (1/3) are metallic. (CNTS) have extraordinary physical characteristics [1, 2].

CNTs have many applications in field emitters, nanosprings, nanoscale electronic devices, and nanbearings [3-7]. Study the bond length between (C- C) and (B-N) are in CNTs and electronic properties are dependent on chirality and diameter [8]. Carbon nanotubes (CNTs) form zigzag (4, 0) are used as a basic computer model, which after substitution with F, Cl and Br, bases simulation of various characteristics. The DFT method is of particular interest for calculating of the molecular structure of CNTs before and after substitution with F, Cl and Br. So, the electronic structure, bandgap, total energy, IR spectrum, Raman spectrum, and depolarization spectrum are calculated using a DFT scheme, that was computed in Quantum program [9].

Using DFT theory to study the effect of iron atom on the band gap, electronic structure for nanotube from (8,0) to (12,0) [10]. Study the effects of carbon atoms on band gap and DOS for (16,0) and (10,10) nanotubes, from this study found the carbon atom led to decrease the bandgap nanotubes [11]. In theory, many methods were employed to study the bandgap and properties, for example, electric fields and chemical doping [12-16].

The aim of this work was to study effects of Cycloepentanes on electronic and spectra properties of nanotubes molecules using DFT functional and the 3-21G basis set.

2. Computational Approach

All the results were done using Gaussian 09 [17]. The structural properties for CNT, CNT-Cyclopentane, CNT-Cyclopentadiene, and NT-Cyclobutane molecules with doping Cyclopentane, Cyclopentadiene and Cyclobutane in CNT have been computed with B3LYP/3-21G level method.

The E^{HOMO} is the highest occupied molecular orbital while the E^{LUMO} is the lowest unoccupied molecular orbital. On the other hand, the E_g calculated by the following equations [18, 19].

$$I = E^{HOMO}$$

$$E = E^{LUMO}$$

$$Eg = (E^{LUMO} - E^{HOMO}) \quad (1)$$

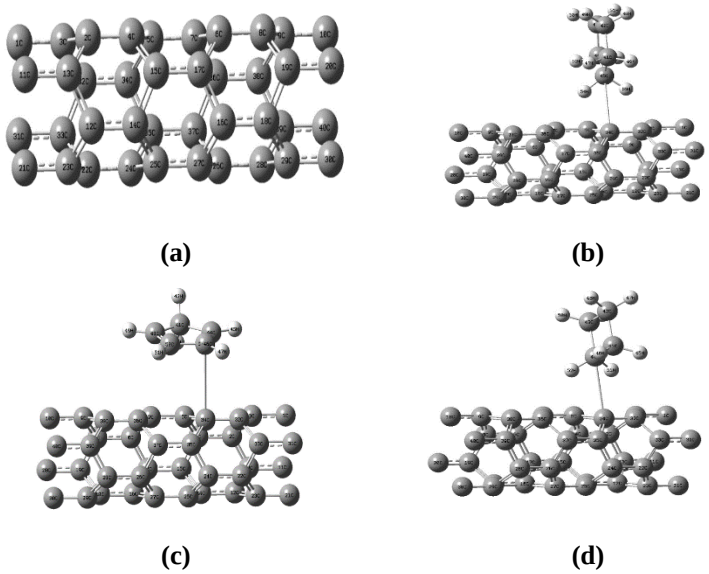
The Fermi energy has been calculated by Eq. (2) [20, 21].

$$E_F = -(I + E)/2) \quad (2)$$

3. Results and Discussion

The correctness of the basis set lies in the consideration of the valence electrons in the bonding and computations. This simulation also takes into account the

polarization and distortion and of the doped CNT molecules. The optimized structures of CNT (A), CNT-Cyclopentane (B) CNT-Cyclopentadiene (C) and CNT-Cyclobutane (D) molecules are calculated by means of DFT/ 3-21G method and it is clearly in Fig. 1.



(a) **(b)**

(c) **(d)**

Fig. 1. The geometric structures of CNT (a), CNT-Cyclopentane (b) CNT--Cyclopentadiene (c) and CNT-Cyclobutane (d) molecules using DFT/ 3-21G method.

3.1. Electronic properties

Table 1 shows the computed parameters such as E^{HOMO} and E^{LUMO} and electronic properties (I, E, E_g, E_f and E_T) for nanotube molecules(A-D) that calculated using DFT with 3-21G basis set are shown in. This table indicates that the E, E_f and E_T are increasing, whereas the LUMO, HOMO, E_g, and I are decreasing, this indicate to the additional reactive molecule in the responses with electrophiles. The CNT-Cyclopentadine system possesses higher *HOMO*, this value rests on doping. the E_g are decreasing for the doping.

The E_g refer to the molecule activity in calculated outcomes and CNT-Cyclopentadine molecule has small E_g 1.245175eV, small E_g directed to molecule the activity, whereas CNT has high E_g 1.456605 eV compare any molecule under study. From our results, all molecules have semiconductor conduct with small bandgap values. From Fig. 2, that the Cyclopentanes change to the *LUMO* values and the *HOMO* vales. Figure 2 shows the charge distribution on along the rings (C-C) and the virus parts of nanotube, all molecules the *HOMO* shows a bonding character and *LUMO* shows antibonding.

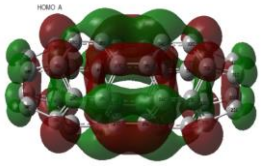
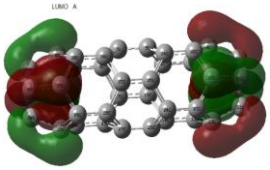
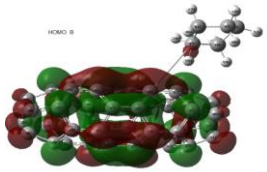
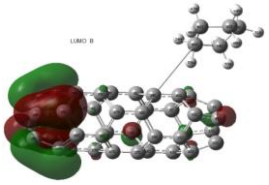
From Table 2, the dipole moments, degree of freedom, Rotational constant, polarizability, Zero-point vibrational, for CNT, CNT-Cyclopentane, CNT-Cyclopentadiene, and CNT-Cyclobutane molecules were computed by means of DFT with 3-21G basis set found are increasing compare CNT, except Rotational constant are decreasing.

Table 1. HOMO, LUMO energies and electronic properties (I, E, E_g, E_f and E_T) in (eV) units for CNT, CNT-Cyclopentane, CNT--Cyclopentadiene, and CNT-Cyclobutane molecules using DFT/ 3-21G method.

Molecules	HOMO	LUMO	I	E	E_g	E_f	E_T
CNT-	-6.05798	-4.60138	6.057985	4.60138	1.456605	5.329683	-1514.66
CNT-Cyclopentane	-5.972	-4.53145	5.971998	4.531448	1.44055	5.251723	-1710.16
CNT-Cyclopentadine	-5.5886	-4.34342	5.588595	4.34342	1.245175	4.966008	-1707.81
CNT-Cyclobutane	-6.07404	-4.61771	6.074039	4.617707	1.456333	5.345873	-1671.03

Table 2. Dipole moments (Debye) , Degree of freedom, Rotational constant (GHZ), polarizability, Zero-point vibrational (J/MOL) for CNT , CNT-Cyclopentane , CNT-Cyclopentadiene , and CNT-Cyclobutane molecules using DFT/ 3-21G method.

Molecules	dipole moments	Degree. of freedom	Rotational constant	polarizability	Zero-pint
CNT-	**0**	**29**	**0.417433**	**239.225**	**586784.1**
CNT-Cyclopentane	**1.3502**	**159**	**0.216741**	**766.256-114**	**965146.3**
CNT-Cyclopentadine	**5.3811**	**147**	**0.245866**	**732.299**	**860522**
CNT-Cyclobutane	**0.2592**	**150**	**0.164361**	**739.007**	**884110.3**

Molecules	HOMO	LUMO
CNT		
CNT- Cyclopentane		

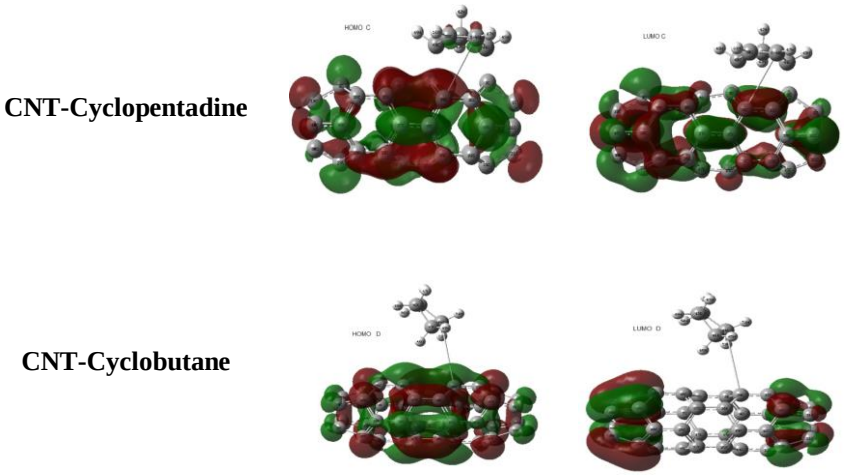


Fig. 2. Shapes HOMO and LOUMO for CNT (A), CNT-Cyclopentane (B) CNT-Cyclopentadiene (C) and CNT-Cyclobutane (D) molecules using DFT/ 3-21G method.

3.2. Density of state (DOS)

Figure 3 illustrates that the DOS of CNT-Cyclopentane (B) CNT-Cyclopentadiene (C) and CNT-Cyclobutane (D) molecules using DFT method with 3-21G basis set. with the adsorption of cyclopentans molecules are different from the corresponding pristine CNT. In the adsorption of Cyclopentanes molecules on CNT, the highest of peaks becomes less, in comparison with pristine CNT, except CNT-Cyclobutane (D) molecules is high, the conduction and valence bands are less with the highest number of density of states.

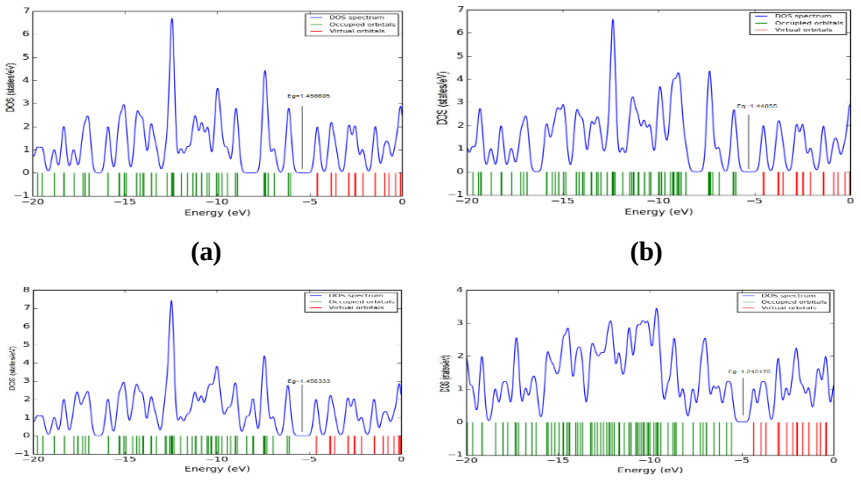


Fig. 3. The density of state of CNT, CNT-Cyclopentane, CNT-Cyclopentadiene, and CNT-Cyclobutane molecules using DFT/ 3-21G method.

3.3. IR spectra

The IR spectra of the (C=C), (C-C) stretching, (C=C=C) out of plane and (C=C) waging studied in the region 1557-67 cm^{-1},1230.95 cm^{-1}, 956.804 cm^{-1} and 689.928 cm^{-1} for CNT, we can see Fig. 4(a), the CNT-Cyclopentane (b) CNT-Cyclopentadiene (c) and CNT-Cyclobutane (d) molecules and the (C-C) studied in the region 1566.28-1625.32 cm^{-1} for pure molecule, we can see from Fig. 4(b)-(d).

The doping leads to deferent vibration modes for molecules understudy. The CNT-Cyclopentane (b) CNT-Cyclopentadiene (c) and CNT-Cyclobutane (d) molecules have (C-H) stretching and (C -H) waging studied in the region 3117.45-3161.61and 1624.67- 1561.56 cm^{-1}, except CNT-Cyclopentadiene (C) has high (C-H) setereching 3247.96 cm^{-1} compare any molecule under. while (C=C) stretching, (C=C=C) out of plane and (C=C) waging for the CNT-Cyclopentane (b) CNT-Cyclopentadiene (c) and CNT-Cyclobutane (d) molecules studied in the region 1229.38-1247 cm^{-1}, 1049.99-1315.5 cm^{-1}, except CNT-Cyclobutane (d) molecules has small value (852.127) cm^{-1}. and (C=C) waging studied in the region 673.644-970.182 cm^{-1}, the CNT -Cyclopentadiene (c) has high(C=C) waging 970.182 cm^{-1} and many peaks vibration harmonic is weak compare any molecule under study.

From this Fig. 4, we can see the effect of Cyclopentans is led to the vibration harmonic are weak.

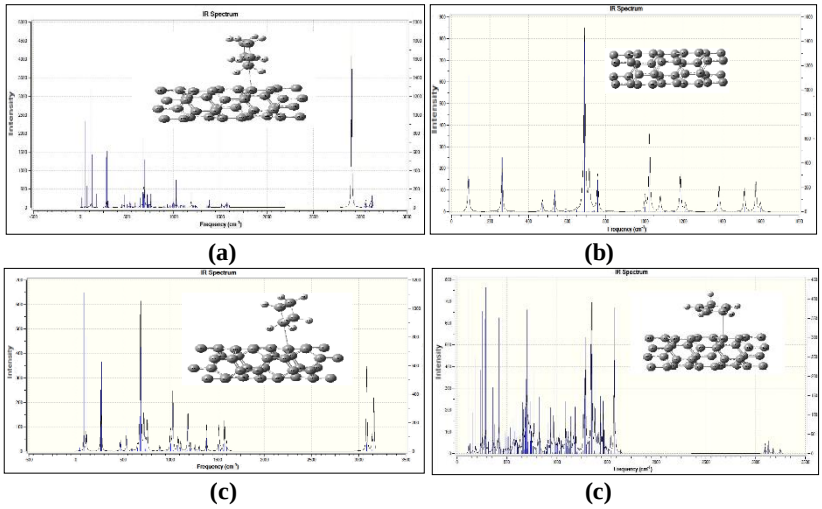


Fig. 4. Shapes IR spectra for CNT (a), CNT-Cyclopentane (b) CNT-Cyclopentadiene (c) and CNT-Cyclobutane (d) molecules using DFT/ 3-21G method.

4. Conclusions

In this study:

- We explored the HOMO, LUMO, E_g, and I are decreasing, while the values of E, E_f and E_T are increasing, The CNT-Cyclopentadine possesses high HOMO, depending on the doping.
- The E_g are decreasing for the doping. CNT-Cyclopentadine molecule has small E_g 1.245175 eV, while the CNT-Cyclobutane has high E_g 1.456333ev, the

deferent of *Eg* refer to the molecule activity, whereas CNT has high E_g 1.456605 eV compare any molecule under study. The values of the property's dipole moments.

- Degree of freedom, rotational constant, polarizability, Zero-point vibrational, for CNT, CNT-Cyclopentane, CNT-Cyclopentadiene, and CNT-Cyclobutane molecules Calculated using DFT 3-21G method found are increasing compare CNT, except Rotational constant are decreasing. The DOS of CNT-Cyclopentane (B) CNT-Cyclopentadiene (C) and CNT-Cyclobutane (D) molecules using DFT/ 3-21G method are different from the CN, we can see the effect of Cyclopentans are led to the changed of vibration harmonic.
- From this research all molecules are very important in many applications.

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