Kuwait J. Sci. **44 (2)** pp. 97-104, 2017

Simulation and calculation of 2, 4, 5, 2′, 4′, 5′ -hexachlorobiphenyl passing from the central axis of single walled carbon nanotube

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Abstract

The 2, 4, 5, 2′, 4′, 5′ -hexachlorobiphenyl (PCB-153) is a high resistant pollutant which cause adverse health effects in recent years. In this study, it is closed and passed into single walled carbon nanotube (8, 8) and is investigated using density functional theory calculations (B3LYP/6-31+G (d)) in terms of complex energy, HOMO/LUMO energy, energy gap (E_g) changes, thermodynamic properties, structural deformation and so on.

The results show that, the PCB-153 around SWNT increased the electrical conductivity and sensitivity of SWNT. Calculated electrical and thermodynamic properties show a sudden change in the middle of the tube, where it may act as a trap for the studied pollutant. The results indicated that the nanotube has considerable ability to interact with PCB-153 and cause it's degradation. Therefore, for detection and reduction of PCB-153, the nano-filter of SWNT can be used. The total Gibbs free energy and other thermodynamic properties show that, these passings from SWNT can be done favorably and spontaneously.

Keywords: B3LYP/6-31+G (d); DFT method 2; single walled carbon nanotube (8, 8); 4, 5, 2′, 4′, 5′ -hexachlorobiphenyl

1. Introduction

Polychlorinated biphenyls (PCBs) comprise a group of 209 synthetic isomers and congeners that differ in the position and number of chloride atoms in the biphenyl structure (Lu *et al.,* 2004). They are the most toxic and toxicity studies have shown that PCB mixtures can cause cancer in experimental animals (Mayes *et al.,* 1998), was banned since the 1970s,This material is very stable and resistant to chemical and biochemical analys is (Ross, 2004). These compounds can transfer from the environment into the organisms and accumulate through the food chains, in the fat tissues (Glauert *et al.,* 2008; Zhu *et al.,* 2009). Today it is uncovered that exposure to the congeners of PCBs could lead to various types of diseases, specially brain disorders and cancers (Steenland *et al.,* 2006; Loomis *et al.,* 1997). Because of above mentioned adverse effects, degradation of these harmful pollutants has been an environmental concern in recent decades. Carbon nanotubes have a very high specific space, high permeability and good mechanical and thermal stability (Thilagavathi *et al.,* 2015). Also, their empty (gash) structure made them very strong with high specific space (Lin *et al.,* 2008). These materials are very resistant to chemicals and have high thermal stability. Since electrons can transfer along the axis of carbon nanotube, they are both electrical and thermal conductive along their axis. They can contain gases and liquids (Tan *et al.,* 2012; Ren *et al.,* 2011). Consequently, using carbon nanotube technology is rather inexpensive in the long run because they can be used without a considerable loss of reduced absorption capacity. Also, carbon nanotube sensors have a potential capability for the monitoring of the environment and can be easily developed for poisons and harmful chemicals (Wang *et al.,* 2009; Pang *et al.,* 2015).

Many theoretical researches have studied the remediation potential of the nanostructures with exposure to various pollutions in aquatic and gaseous phases (Long & Yang 2001). In this study, it is investigated to identify and remove the pollution of chlorinatedaromatic compounds by single wall carbon nanotubes. Figure 1 shows the optimized geometrical structure PCB-153 and SWNT (8, 8) by GAMESS program package based on B3LYP/6-31+G(d).

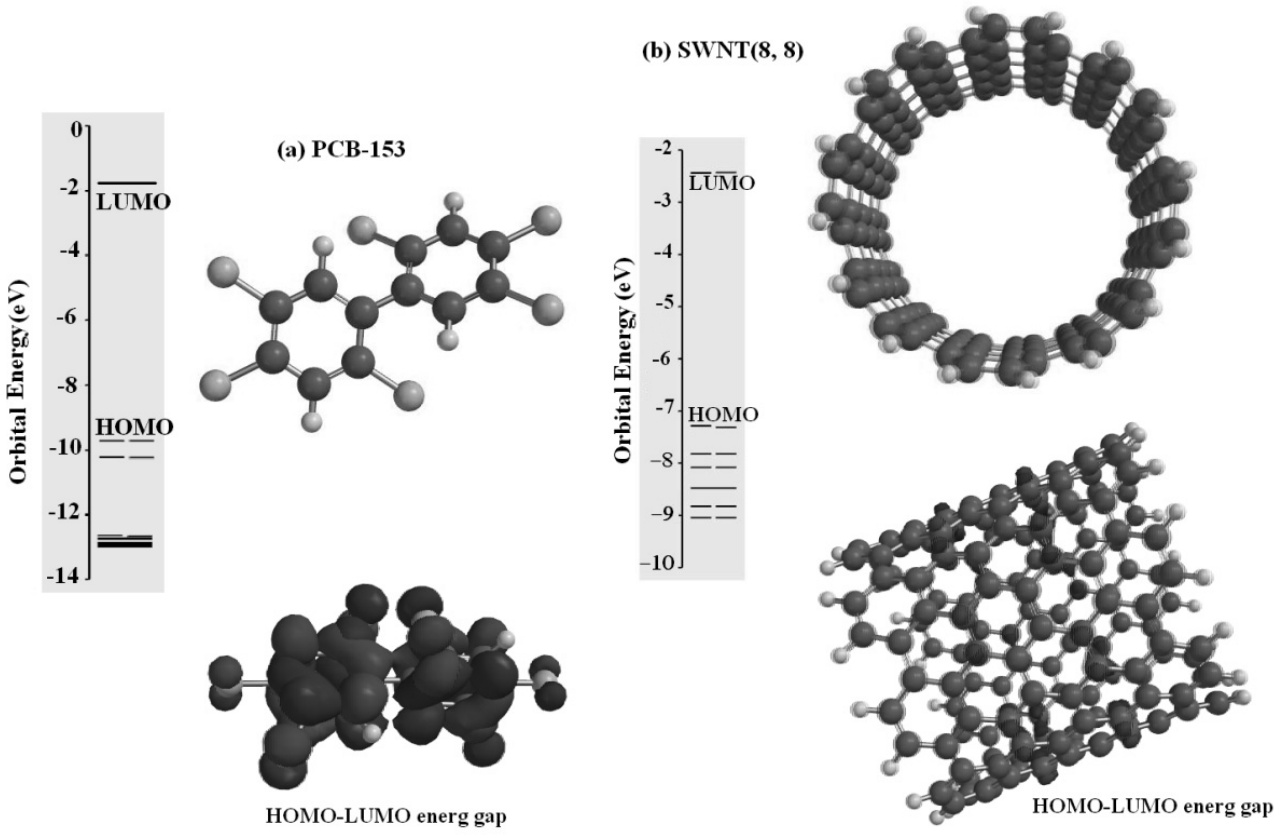

Fig. 1. The ball and stick model of optimized geometrical structure: a) PCB- 153, b) single wall carbon nanotube (8, 8) with HOMO and LUMO energy of them.

Both ends of the carbon nanotube are closed by hydrogen atoms. After being optimized SWNT and PCB-153, the passing of PCB-153 from the central axis of carbon nanotubes (Figure 2) is simulated and the electrical and thermodynamic properties of such interactions are calculated by B3LYP/6-31+G(d). In this study, the interaction of 2, 4, 5, 2′, 4′, 5′ -hexachlorobiphenyl (PCB-153) with SWNT(8, 8) will be theoretically investigated, based on analyses of structure, energies, HOMO-LUMO gaps (E_g), stability, electrical and thermodynamic properties and so on. Our results are likely to be useful for further studies related to make of SWNT(8, 8): as a nano-filter.

2. Computational method

First of all a single wall carbon nanotube (8, 8) is formed by nanotube modeler package (www.jcrystal.com/products/wincnt/nanotube). Then 2, 4, 5, 2′, 4′, 5′ -hexachlorobiphenyl (PCB-153) is simulated by Chemoffice package. Both their structures and complex caused by pollutant passing from the central axis of carbonnano tubes (Figure 2) are optimized using B3LYP exchange-functional and applying basis set 6-31+G(d) by GAMESS program package (Schmidt *et al.,* 1993) working under Linux. Molecular properties such as geometries, energies and vibrational frequencies were calculated by this method. By obtaining parameters of the simulated interaction, calculation of the thermodynamic parameters will be possible. It should be noted that the passing of PCB within nanotube was simulated in room temperature and at five distances.

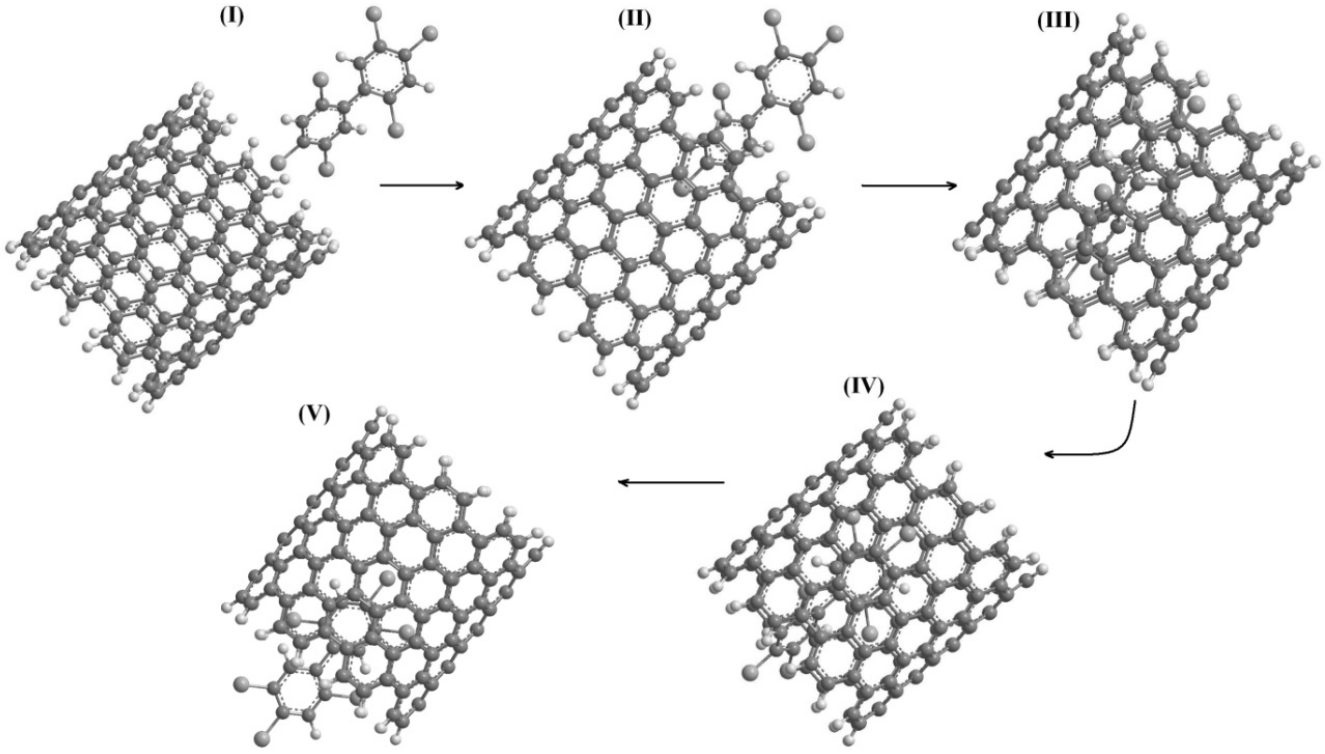

Fig. 2. The steps of the proposed reduction mechanism of PCB-153 passing intro SWNT (8,8) by B3LYP/6-31+G(d) method.

The complex energy (E_c) of all steps of 2, 4, 5, 2′, 4′, 5′ -hexachlorobiphenyl passing into SWNT (8, 8) has been calculated as follows:

$$E_c = E_{\text{PCB-153-nanotube}} - [E_{\text{PCB-153}} + E_{\text{nanotube}}] + \delta_{\text{BSSE}} \quad (1)$$

Where $E_{\text{PCB-153-nanotube}}$ is the passing energies of PCB-153 and SWNT (8, 8), $E_{\text{nanotube}}$is the energies of the SWNT, $E_{\text{PCB-153}}$ is representing the energy of an isolated PCB-153 molecule and δ_{BSSE} is representing the basis set superposition error.

3. Results and discussion

For the interaction between 2, 4, 5, 2′, 4′, 5′ -hexachlorobiphenyl (PCB-153) and single wall carbon nanotube, there are many probabilities such as: adsorption on top of the nanotube, the adsorption of the wall of nanotube, passing through the central axis nanotube without interaction with the wall or interaction with the inside wall of a nanotube. In this study passing of PCB-153 through the centralaxisnanotube without interaction with the wall of nanotube is investigated. The complex energy (E_c/kJ.mol^{-1}) for all steps is calculated according to Equation (1), as shown in Figure 3. Figure 3 shows a significant decrease in the 3rd step (center of nanotube). Other parameters of thermodynamics for this interaction is indicated in Table1.

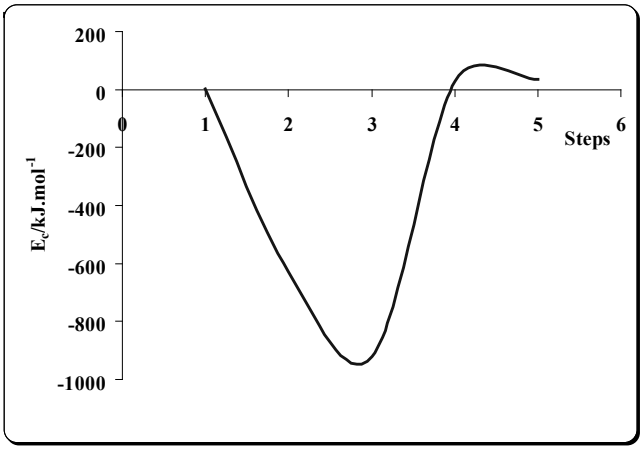

Fig. 3. The complex energy (kJ.mol^{-1}) of PCB-153 passing across from SWNT (8, 8).

Based on Table 1, the passing of the PCB-153 across from the nanotube in first step increases the total energy, then in the middle of the tube length, the slope decreases significantly. Therefore, the center of the tube is a place for the entrapment of PCB-153. Increasing of the total energy again at the end of the nanotube, shows that can be outside pollutants from carbon nanotubeandtobe recycled nanotube by increasing of the temperature**.**

Table 1. The calculation of total energy (E_{total}), Dipole moment (DM), Zero point energy (ZPE), heat of reaction formation (H^o), Gibbs free energy (G^o), heat capacity (C_v) and entropy (S^o) forSWNT (8, 8), PCB-153 and steps of passing of PCB-153 intro SWNT at the B3LYP/6-31+G(d) method.

	SWNT (8, 8)	PCB-153	I	II	III	IV	V
E_{total}/kJ.mol^{-1}	3704.20	61.18	3768.24	3138.12	2845.71	3795.54	3799.52
Dipole Moment/D	0	0.04	1.50	1.04	1.00	1.33	1.48
E_{ele}/kV	436.28	0.12	566.29	595.51	614.60	624.08	617.94
ZPE/kJ.mol^{-1}	3858.77	326.97	4200.60	4080.34	4001.09	4200.55	4200.83
H^o/kJ.mol^{-1}	2.946	0.16	3.11	2.83	2.56	3.12	3.10
G^o/kJ.mol^{-1}	2.804	0.11	2.95	2.66	2.12	2.96	2.94
C_V/J.K^{-1}.mol^{-1}	1126.11	175.62	1295.90	1335.10	1296.02	1296.02	1294.31
S^o/J.K^{-1}.mol^{-1}	1249.67	500.95	1468.60	1517.34	1576.52	1463.46	1460.25

Most of the changes are indicated in middle nanotube, the dipole moment of SWNT increases at first until third step decreases, because this step is more symmetric complex structure. Zero point energy (ZPE) has less among in 3rd step, is 4001.09 kJ.mol^{-1}. The heat of reaction formation (H^o) and Gibbs free energy (G^o)/kJ.mol^{-1} decrease in the middle length of the nanotube, because nanotube tends to take PCB-153 into itself, this passing is exothermic. The heat capacity (C_v) and entropy (S^o) shown at, the central part of the nanotube is a suitable location for the adsorption of pollutant.

Table 2 shows the highest occupied molecular orbital (HOMO) and the lowest un-occupied molecular orbital (LUMO) energy for the pristine of SWNT (8, 8) andPCB-153, the energy gap (E_g) of them are 4.85eV and 8.62eV, respectively. They are an insulating material and are stable (due to their large HOMO-LUMO gap). Characteristics such as the width of the valence band, the gap energy in insulators and the number and intensity of the main features are helpful in qualitatively interpreting experimental spectroscopic data. Table 2 shows its parameters including E_{LUMO} (energy of the lowest unoccupied molecular orbital), E_{HOMO} (energy of the highest occupied molecular orbital), E_g (gap energy), μ (chemical potential or the negative of electronegativity), η (chemical hardness), σ (chemical softness), ω (electrophilicity) and ΔN_{MAX} (charge transfer in molecules) (Ahmadi & Pirahan-Foroush 2014a), are calculated by B3LYP/6-31+G(d) in DFT method.

$$\mu = (E_{LUMO}+E_{HOMO})/2 \quad (2)$$

$$\eta = (E_{LUMO}-E_{HOMO})/2 \quad (3)$$

$$\sigma = 1-\eta \quad (4)$$

$$\omega = \mu^2/2\eta \quad (5)$$

$$\Delta N_{MAX} = -\mu/\eta \quad (6)$$

The gap energy (E_g) is a major factor for the determination of the electrical conductivity of nano-materials. If the calculated amount of E_g for complexes is most, sensitivity and conductivity between them will be considerable and nanostructure can be used as nano-sensors.

In studying interactions, the least amountof gap energy occurred for 3rd step, because the SWNT-PCB has symmetry and the polarity of them increases. According to table 2, the chemical potential (μ) increases in 3rd step, indicating a transfer of electrons from PCB-153 to SWNT molecule. The chemical hardness (η) and chemical softness (σ) are used for evaluation of the hardness and softness of molecules. Hard molecule has a large HOMO-LUMO gap, while a soft molecule has a small HOMO-LUMO gap (Ahmadi & Pirahan-Foroush 2014b).

Table 3. The electronic parameters calculation for SWNT (8, 8), PCB-153 and staps of passing of PCB-153 intro SWNT at the B3LYP/6-31+G(d) method.

	SWNT (8, 8)	PCB-153	I	II	III	IV	V
E_{HOMO}/eV	-7.29	-9.27	-7.28	-7.36	-5.23	-7.31	-7.30
E_{LUMO}/eV	-2.44	-0.65	-2.44	-2.47	-0.86	-2.47	-2.41
E_g/eV	4.85	8.62	4.84	4.89	4.37	4.84	4.89
μ/eV	-4.87	-4.96	-4.86	-4.92	-3.05	-4.89	-4.86
η/eV	2.43	4.31	2.42	2.45	2.18	2.42	2.45
σ/eV	-1.43	-3.31	-1.42	-1.45	-1.18	-1.42	-1.45
ω/eV	4.88	2.85	4.88	4.94	2.12	4.94	4.82
ΔN_{MAX}/eV	2.01	1.16	2.01	2.01	1.39	2.02	1.99

Therefore 3rd step is harder than other states and can easily change their electron density. The electrophilicity (ω) is a measure of the electrophilic power of a molecule. The ω value isdecreasing toward 3rd step, which shows higher electrophilicity than other steps. So it is a stronger Lewis base. The accepted and donor electron charge of molecules can be calculated by a maximum amount of electronic charge (ΔN_{MAX}). The ΔN_{MAX}<o indicates the molecule acts as an electron donor (Ahmadi & Pirahan-Foroush 2014a). In all steps, SWNT and PCB-153 are electron acceptors and have significant power of electron affinity which can be used for identification of PCB-153.

Broad interpretation is essentially a "sensitivity analysis" of these interactions and it has presented a method to measure the important property of the descriptor in quantitative structure-activity relationship (QSAR) model. The parameters calculated for these interactions by QSAR method are Area/Å^3 (molecular surface area), Volume/Å^3, PSA/Å^2 (polar surface area), Ovality is described by a ratio of volume to area, Acc.Area/Å^2 (Accessible area), P-Area/Å^2 (polar area corresponding to absolute values of the electrostatic potential greater than 75), Acc.P-Area(75)/Å^2 (Accessible polar area corresponding to absolute values of the electrostatic potential greater than 75), Min.Elpot/kJ.mol^{-1} (minimum energy of ionization potential), Max.Elpot/kJ.mol^{-1} (maximum energy of ionization potential), Min.LocIonPot/kJ.mol^{-1}(minmum values of the local ionization potential (as mapped on to an electron density surface) and polarizability, as shown in Table 3 (Hehre Warren, 2008).

Table 3. The QSAR calculated for SWNT (8, 8), PCB-153 and steps of passing of PCB-153 intro SWNT at the B3LYP/6-31+G(d) method in 298K.

Steps	SWNT (8, 8)	PCB-153	I	II	III	IV	V
Area/Å^2	1266.72	280.96	1549.64	1526.65	1491.26	1506.60	1546.45
Volume/Å^3	1712.60	260.78	1977.40	1967.65	1954.28	1973.84	1974.76
PSA/Å^2	0	0	0	0	0	0	0
Ovality	1.83	1.42	2.03	2.01	1.76	1.98	2.45
Acc.Area/Å^2	986.65	368.55	1154.84	1131.84	853.22	880.13	1157.63
P-Area(75)/Å^2	1169.11	461.18	1415.81	1414.80	1357.96	1392.20	1426.36
Acc.P-Area(75)/Å^2	986.65	368.55	1154.85	1131.84	853.12	880.14	1175.24
Min Elpot/kJ.mol^{-1}	48834.47	-540894198.14	36793.88	38714.18	42123.54	54082.22	40123.89
Max Elpot/kJ.mol^{-1}	75630.86	-267041908.83	81013.74	82415.38	78963.27	92528.08	84326.87
Min LocIonpot/ kJ.mol^{-1}	197.15	0	99.18	162.98	68.38	99.36	99.19
Polarizability	179.40	60.50	40.23	40.22	40.19	40.23	40.23

The polar surface area/Å^2 (PSA) of a molecule is currently defined as the surface sum over all polar atoms, primarily carbon and hydrogen, which shows the critical role of the charge and polarity of the molecules, In this interaction, there are no polar surface area or Min and Max Elpot of calculating for PCB-153. Hence, they are the most toxic. The results show a significant decreasing of toxicity in the third step. The polarizability of a molecule, an important physical property, is currently attracting our attention, particularly in the area of QSAR for chemical and biological interactions (Verma & Kurup, 2005). All the parameters indicate that 3rd step is conducive to activity for adsorption of PCB-153 to inner SWNT.

The conductance of nanotube is increasing, when PCB-153 is passing across from the nanotube as in the 3rd step is at the top. In other words, PCB passing through nanotube enhances nanotube conductivity. These variations in electrical properties suggest that this nanostructure is able to detect PCB-153 in the environment. The electrical resistance was calculated by the conductivity as:

$$E_{elec} = RI \quad (7)$$

Where E_{elec}(V) is electrical energy, I (A) is electrical intensity and R (Ω) is electrical resistance. The electrical resistance is calculated by:

$$R = \frac{E_{ele}\, t}{n.\mathrm{F}} \quad (8)$$

Where n, F and t are number of exchangeelectrons, Faraday's constant and time (h) of interaction respectively. By obtaining values for the resistivity, the electrical resistance- time graph was drawn as is displayed in Figure 4.

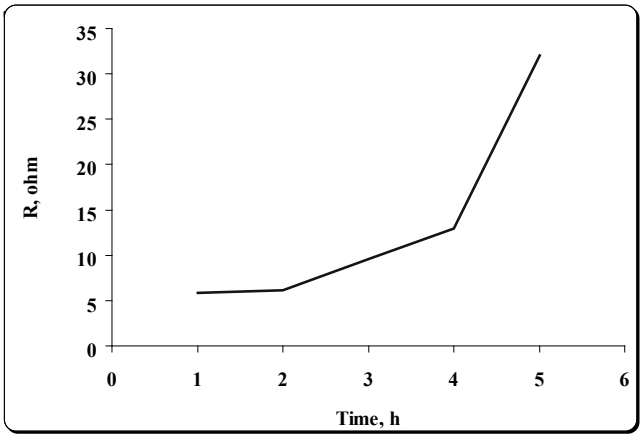

Fig. 4. The electronic resistance (Ω) calculated for passing PCB-153 through SWNT (8, 8).

According to Figure 4 with the entry of the pollutant into the tube, the electrical resistance of the tube decreases and that means an increase of conductivity. Thermodynamic parameters including the Gibbs free energy, enthalpy and entropy differences for 3rd step are calculated using the data in Table 4.

Table 4. The thermodynamic properties of PCB-153 passing acrossSWNT (8, 8) at 298K.

ΔG kJ.mol^{-1}	ΔH k.mol^{-1}	ΔS J.K^{-1}.mol^{-1}	*lnK*
-0.794	-0.546	0.83	0.320

The ΔG and ΔH are negative, so study of passing process is spontaneous. As the entropy is positive, its effect in investigating the interaction is not remarkable. Consequently, passing of PCB-153 through armchair SWNT (8, 8) is favorable in the presence of a little external heat.

4. Conclusion

PCBs are highly toxic compounds and are considered dangerous (Srinivasan *et al.,* 2001). It is noteworthy that the identification, quantitative determination, and ultimate elimination and reduction are the main goals of this research. In this study, simulation and calculation of the thermodynamic parameters for interaction of 2, 4, 5, 2′, 4′, 5′ -hexachlorobiphenyl (PCB-153) with SWNT (8, 8) is investigated. The complex structureof PCB-153 passing into SWNT was optimized by the DFT method with basis set B3LYP/6-31+G (d). The results of calculations show that SWNT has tendency to enter the PCB-153in its central axis and show significant changes in the electrical and thermodynamic properties when PCB-153 into nanotube and most of these changes have been achieved in the middle of nanotube.The data are calculated by QSAR method what indicated that toxicity has decreased for PCB-153 in SWNT.

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Submitted **:** 31/08/2015
Revised **:** 18/04/2016
Accepted **:** 26/04/2016

محاكاة وحساب 2، 4، 5، ′2، ′4، ′5 سداسي كلور ثنائي الفينيل الذي يمر عبر المحور المركزي للأنابيب النانوية الكربونية أحادية الجدار

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خلاصة

2، 4، 5، ′2، ′4، ′5 سداسي كلور ثنائي الفينيل (PCB-153) عباره عن مادة ملوثة ذات مقاومة عالية تسببت في آثار صحية ضارة في السنوات الأخيرة. في هذه الدراسة، يتم إغلاقها وتمريرها في أنابيب نانوية كربونية أحادية الجدار (8، 8)، وتم فحصها باستخدام حسابات نظرية الكثافة الوظيفية ((B3LYP/6-31+G (d) من حيث الطاقة المركبة وطاقة هومو / لومو (HOMO/LUMO) وتغيرات فجوة الطاقة (Eg) والخصائص الحرارية والتشوه الهيكلي وهكذا.

وتُظهر النتائج أن مرور ثنائي الفينيل متعدد الكلور PCB-153 عبر الأنابيب النانوية الكربونية أحادية الجدار، قد زاد من التوصيل الكهربائي وحساسية الأنابيب النانوية الكربونية أحادية الجدار. وتُظهر الخواص الكهربائية والحرارية المحسوبة حدوث تغيير مفاجئ في منتصف الأنبوب، حيث يمكن أن تكون بمثابة مصيدة للملوثات التي تتم دراستها. وأشارت النتائج أن الأنابيب النانوية لديها قدرة كبيرة على التفاعل مع ثنائي الفينيل متعدد الكلور PCB-153 مما يؤدي إلى تحللها. ولذلك، يمكن استخدام فلتر نانو للأنابيب النانوية الكربونية أحادية الجدار من أجل الكشف عن ثنائي الفينيل متعدد الكلور PCB-153 والحد منه. ويبين إجمالي طاقة جيبس (Gibbs) الحرة والخصائص الحرارية الأخرى أنه يمكن إجراء التمريرات عبر الأنابيب النانوية الكربونية أحادية الجدار بشكل إيجابي وتلقائي.