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DFT/NBO study of Nanotube and Calixarene with anti-cancer drug

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Abstract

Nowadays use of calixarenes and nanotubes are widely spread in the pharmaceutical industry. In this work, interaction of between calix[4]arene and nanotube (6, 6) with Fluorouracil drug are investigated. The DFT calculations have been performed using the Gauss view and Gaussian98 in B3LYP method and 6-31G (d) standard basis set at 298.15K. There are calculated length bond (Å), bond angel (deg), dihedral angel (deg), energy hyperconjucation, and total energy (KJ mol^{-1}), moment dipole (Debye), occupancy between nanotube (6, 6) and calix[4]arene with anticancer drug in B3LYP/6-31G (*d*) method. These cases and medicines show that complex1 is more stable than complex1. The parameter of E^2, gap energy and $\Delta E°$ in composite of nanotube- Fluorouracil are higher than calix[4]arene-Fluororacil; therefore, complex1is more stable.

Keyword: Drug delivery; Nanotube; DFT; Fluorouracil; Calix[n]arene; NBO; Capacity heat; Formation energy

Introduction

The application of nanotechnology in disease treatment, diagnosis, monitoring, and in the control of biological systems at the single molecule or molecular assembly level is referred to as nanomedicine. The major goal of nanomedicine is the design of material capable of delivery and targeting of pharmaceutical, therapeutic, and diagnostic agents [1-5]. The type of drug delivery system carbon nanotube discovery by Iijma in 1990_S [6]. A nanotube can be thought of as a hexagonal network of carbon atoms that has been rolled up to make aseamless cylinder [7,8]. Carbon nanotubes exhibit superior thermal [9], mechanical [10], and electrical properties [11] and are considered the most promising building block for manufacturing low-cost, high-performance nanostructured composite materials [12].

In the paper, complexation of between fluorouracil and nanotube (6,6)/calix[4]arene are investigated as drug delivery system. Calixarenes, crown ether, and cyclodextrin are group of organic macrocyclic agents that have cup like shape which are easily available through the cyclocondensation of para-substituted phenols with formaldehyde [13,14]. One way to increase the aqueous solubility of drugs is to use complexing agents to form hast- guest complexes [15-17]. Calixarenes are promising materials for nanomedicine application in drug delivery systems. For example, hydrophilic derivatives have shown interesting levels of activity against bacteria [19], fungi, cancerous cells and enveloped viruses, but also against thrombosis or fibrosis diseases [10,20-22]. Anticancer genes act in a dominant fashion: when ectopically over expressed, they specifically destroy tumor cells without harming normal cells. This cell destruction can come in various modes such as apoptosis, mitotic catastrophe followed by apoptosis or necrosis, and autophage. Anti-cancer genes have only recently emerged from studies on cancer cells [23-26]. Fluorouracil or 5-Fluoropyramidin-2,4(1H, 3H)-dion is used as anticancer drug. Fluorouracil is an analog of pyrimidine which has been used as an anti-cancer drug for 40 years. The structure of fluorouracil is observed in Figures 1a and 2. It is anti metabolite drug and acts in several ways, but principally as synthesis inhibitor. These days there are ways to deliver a drug in the body without side effects [27]. In this paper, we reported types of drug delivery system such as nanotube and calix[4]arene.

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Results and discussion

The several computational tools of, such as Density Functional Theory (DFT), Car-Parrinello molecular dynamics

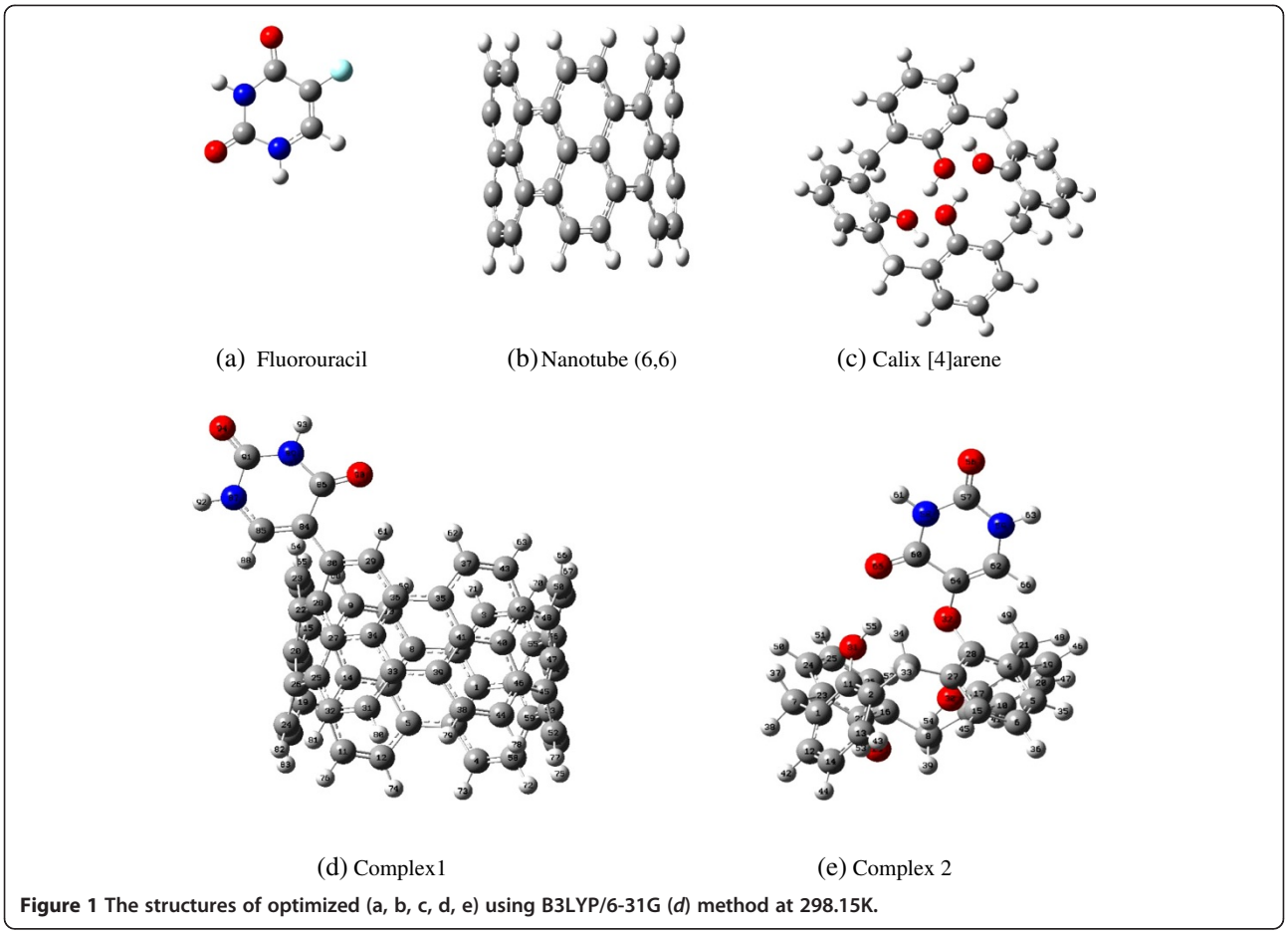

Figure 1 The structures of optimized (a, b, c, d, e) using B3LYP/6-31G (*d*) method at 298.15K.

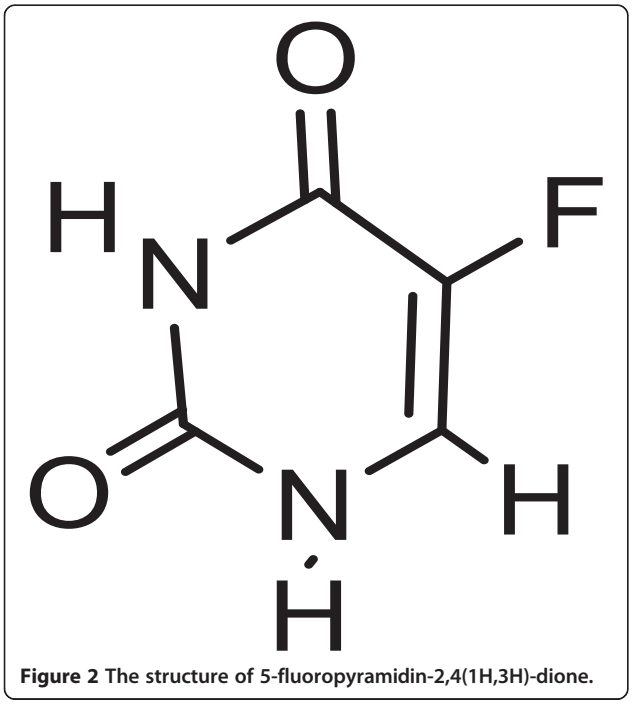

Figure 2 The structure of 5-fluoropyramidin-2,4(1H,3H)-dione.

simulations, and hybrid QM/MM approaches, can be used for calculations. Density functional quantum chemical calculations have recently provided a relatively consistent picture on base pair interaction energies and geometrics. This can lead to more detailed information on structure, charge distribution, and energetic of the base pair [28-31]. At present, quantum chemical is almost universally applicable to the interpretation of physical and chemical properties of various compounds [32]. Understanding the biochemical mechanism of a disease usually suggests the types of molecules required for new drugs. In all cases, the aim of using the computer for drug design is to analyze the interactions between the drug and receptor sites and to design drugs that give an optimal fit [33-35]. Figure 1 shows the optimized compound calix[4]arene, nanotube (6,6), fluorouracil, nanotube (6,6)-fluorouracil (complex 1), and calix[4]arene-fluorouracil (complex 2) by DFT method in level B3LYP/6-31G (*d*).

The highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), [36], the HOMO-LUMO bond gap have been found as a measure of the structural stability properties [37]. The parameters of bond length (Å), natural bond orbital (NBO) and bond angle (deg), dihedral angle (deg),

Table 1 Parameters of in B3LYP/6-31G (*d*) method optimized by complexes 1 and 2 at 298.15K

Agent	Complex 1	Complex 2
$C_{30}-C_{84}/O_{84}$	1.47	1.40
$C_{30}=C_{20}$	1.37	1.35
$C_{36}\equiv C_{29}$	1.43	1.40
$C_{28}-C_{30}$	1.47	1.46
$C_{85}\equiv N_{87}$	1.37	1.38
$N_{87}-C_{91}$	1.39	1.40
$C_{91}=O_{94}$	1.22	1.23
$C_{30}-C_{28}\equiv C_{27}$	116.02	121.62
$C_{84}=C_{85}-H_{88}$	121.36	122.70
$C_{85}\equiv N_{87}-H_{92}$	120.82	120.48
$N_{87}-C_{91}=O_{94}$	123.42	123.77
$C_{91}-N_{89}-H_{93}$	115.60	115.47
$O_{90}=C_{86}-C_{84}$	126.90	124.39
$C_{30}-C_{84}=C_{85}\equiv N_{87}$ [1]	178.86	-
$H_{87}-C_{84}-N_{86}\equiv H_{91}$ [2]	0.79	0.52
$C_{90}-N_{88}-C_{85}=O_{89}$ [3]	−178.64	−179.12
$H_{61}-C_{29}=C_{30}-C_{28}$ [4]	172.74	-
$O_{94}=C_{91}-N_{89}-C_{86}$ [5]	179.16	173.95
$C/H_{30}-C_{28}\equiv C_{27}\equiv C_{34}$ [6]	−26.01	35.84

Bond distances (Å), Bond Angles (deg) and dihedral Angles (deg).
1: $C_{30}-C_{84}=C_{85}\equiv N_{87}$ dihedral angles, 2: $H_{87}-C_{84}-N_{86}\equiv H_{91}$ dihedral Angles, 3: $C_{90}-N_{88}-C_{85}=O_{89}$ dihedral Angles, 4: $H_{61}-C_{29}=C_{30}-C_{28}$ dihedral angles, 5: $O_{94}=C_{91}-N_{89}-C_{86}$ dihedral angles, 6: $C/H_{30}-C_{28}\equiv C_{27}\equiv C_{34}$ dihedral angles.

distances of analysed models of the nanotube (6, 6) and calix[4]arene are calculated by DFT at the level of B3LYP and 6-31G (*d*) standard basis set and are shown in Table 1. The DFT calculated geometric parameters for complex 1, and 2 are compared in Table 1. The bond lengths C_{30}-C_{84}/O_{84} calculated for complex 1, 2 at the DFT level range from 1.47 to 1.40 Å, at the B3LYP/6-31G (*d*) level.

The bond lengths calculated at $C_{36}\equiv C_{29}$ for complex 1 (in ring nanotube), 1.44 Å and, for complex 2, 1.40 Å, are within the range (in ring calixarene). The bond lengths calculated $C_{85}\equiv N_{87}$ for complex 1, 1.37 Å, and complex 2 are ranged 1.38 Å. The $C_{88}\equiv N_{92}$ bond length is lower than $C_{36}\equiv C_{29}$ bond length in complex 1 and 2. With that reason, there is more electronegativity of nitrogen than carbon.

The angles for N_{87}-$C_{91}=O_{94}$ are 123.41° and 123.77° for complexes 1 and 2. The angles for C_{84}-$C_{86}=O_{90}$ are 126.9° and 124.4° for complex 1, 2. The angles for C_{84}-$C_{86}=O_{90}$ is larger than the angel for N_{87}-$C_{91}=O_{94}$ in complexes 1 and 2. The interaction of between nonbonding and bonding pairs on the nitrogen atom of the angle are reduced in N_{87}-$C_{91}=O_{94}$.

The dihedral angles for C/H_{30}–$C_{28}\equiv C_{27}\equiv C_{34}$ for complex 1 and 2 range from −26.01° to 35.84° (in dihedral 6). The dihedral angles 1,2,3,4,5 and 6, are observed in Table 1 and Figure 3.

The calculations of the total energies, hyperconjoucation energy (E^2) of the optimized structures, dipole moments (μ), occupancy and hybrid at B3LYP/6-31G (*d*) levels are presented in Tables 2 and 3. In Table 2, the Mulliken charges in donor atoms electronegative O_{84} and acceptor

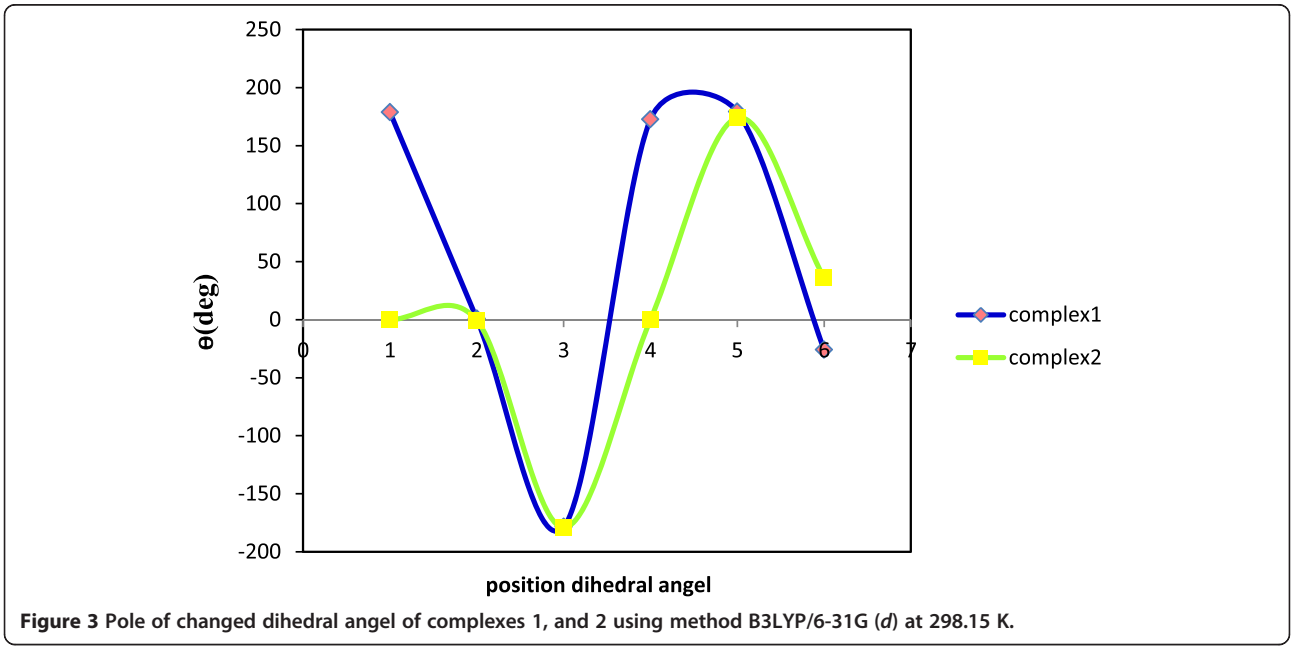

Figure 3 Pole of changed dihedral angel of complexes 1, and 2 using method B3LYP/6-31G (*d*) at 298.15 K.

Table 2 The NBO parameters of, Complex 1 and 2 are calculated in B3LYP/6-31G (*d*) method at 298.15K

Agent	Donor	Occupancy	Acceptor	Occupancy	hybrid	E^2	ΣE^2
Complex1	BD(1)C30- C84	1.96631	BD*(1)C27-C28	0.02586	$SP^{1.98}$	1.48	35.53
			BD*(1)C28-C30	0.02920	$Sp^{2.06}$	1.70	
			BD*(1)C29-C30	0.02033	$Sp^{1.79}$	3.12	
			BD*(1)C29-C36	0.02164	$SP^{1.96}$	2.51	
			BD*(1)C84-C85	0.01852	$SP^{1.88}$	3.55	
			BD*(1)C84-C86	0.06682	$SP^{2.28}$	1.82	
			BD*(1)C85-N87	0.01939	$SP^{2.51}$	3.76	
	BD*(2)C84-C85	0.23733	BD*(2)C29-C3	0.2195	$SP^{99.99}$	17.59	
Complex2	BD(1)C28-O32	1.94416	BD*(1)C4-C5	0.0219	$SP^{1.9}$	1.48	22.77
			BD*(1)C15-C27	0.02108	$SP^{1.85}$	1.6	
			BD*(1)C60-C64	0.07182	$SP^{1.71}$	1.93	
			BD*(2)C62-C64	0.24487	$SP^{1.00}$	0.66	
			BD*(1)C4-C28	0.03327	$SP^{1.98}$	1.88	
	LP(1)O32	1.93171	BD*(2)C27-C28	0.37632	$SP^{1.00}$	5.18	
			BD*(1)C4-C28	0.03327	$SP^{1.98}$	3.86	
	LP(2)O32	1.87683	BD*(1)27-C28	0.03258	$SP^{1.95}$	6.15	

C_{30} are negative and positive, respectively. Complex 1 has gap of energy that is larger than complex 2; therefore, complex 1 is stable. In Table 2, it becomes obvious that the complex 1 has formed higher hyperconjugation energy than complex 2. Also, the results show that by increasing P part in hybrid of atoms, the occupancy decreases. The S orbital part in hybrid of carbon in complex 2 is more than the S orbital part in hybrid of in complex 1. Combined with the most of hyperconjugation energy is stable. The occupancy coefficient is smaller. Complex 1 is more stable than the complex 2. The hyperconjugation energy complex 1 at 37.34 is larger than that in complex 2. The hybrid orbital S of a compound is lower. Table 2 shows the HOMO and LUMO energies for complexes. By evaluating HOMO/LUMO gap energies, it is obvious that if the gap becomes bigger, the complex will be stable; therefore, complex 1 is more stable than the complexes. The results of the present work were obtained using DFT optimization and formation energy (ΔE°_{f} in $KJmol^{-1}$) calculation at the B3LYP/6-31G (*d*) level. ΔE°_{f} is calculated using the formula $\Sigma E^{\circ}{}_{\text{product}} - \Sigma E^{\circ}{}_{\text{reactant}}$. ΔE°_{f} values in complexes 1 and 2 are in the range of −13.275 and +46.902 $KJmol^{-1}$; therefore, complex1 has lower formation energy than the others. The energy (kJ mol^{-1}) and dipole moments (Debye) indicate the consistency between the two complex calculations in DFT method. The gap energies and total energy, ΣE^2, HOMO and LUMO complexes 1, 2 were calculated using the B3LYP method and 6-31G (*d*) basis set. The total energy sum of energy transitional, energy rotational and energy vibration in level B3LYP/6-31G (*d*) for complexes 1, 2 was calculated. The obtained results are shown in Table 3.

Heat capacity is the measurable physical quantity that specifies the amount of heat required to change the temperature of body by a given amount. Translation, rotation, and a combination of the two types of energy in vibration (kinetic and potential) of atoms represent the degrees of freedom of motion which classically contribute to the heat capacity of matter, but loosely bound electrons may also participate. On a microscopic scale, each system particle absorbs thermal energy among the few degrees of freedom available to it, and at sufficient temperatures, this process contributes to the specific heat capacity that classically approaches a value per mole of particles that is set by the Dulong-Petit law. For quantum mechanical reasons, at any given temperature, some of these degrees of freedom may be unavailable, or only partially available, to store thermal energy. Quantum theory can be used to quantitatively predict the specific heat capacity of simple systems.

Table 3 Formation energy, total energy, HOMO, LUMO, Gap of energy, moment dipole and heat capacity are calculated in B3LYP/6-31G (*d*) method at 298.15 K

Agent	E_{total}	ΔE°_{f}	HOMO	LUMO	Gap	μ	C_V
Complex 1	465.73	−13.275	−0.15877	−0.08918	−0.0696	0.527	191.03
Complex 2	348.03	+46.902	−0.19989	−0.05481	−0.14508	0.591	130.52

Conclusions

In this paper, the result shows that complex 1 between Nanotube (6,6) and fluorouracil is more stable than complex 2. Thus, complex 1 is a better conditioner for drugs than complex 2. NBO analysis shows larger gap energy in complex 1. Complex 1 has lower formation energy and is more stable than complex 2.

Methods

Investigation is carried out using a personal computer (Intel (R) Pentium (R) dual CPU with 2GB RAM). Nanotube-fluorouracilarene (with different atom number) which reacts with anti-cancer drug. In this paper, the drug delivery properties are investigated by NBO analysis and DFT method. The DFT calculations have been performed using the Nanotube modeler [38], Gaussview [39] and Gaussian 03 [40] using B3LYP method and 6-31G (*d*) standard basis set. NBO analysis [41,42] calculations have been also performed for all composites using B3LYP method and the standard 6-31G (*d*) basis set. Complexes between calix[4]arenes and nanotube (6,6) with Fluorouracil drug are optimized, then bond length (Å), bond angel (deg), dihedral angel (deg), hyperconjucation energy, as well as total energy ($KJmol^{-1}$), moment dipole (Debye), occupancy, total energy and HOMO/LUMO are investigated between nanotube (6, 6) and calix[4]arene with anti-cancer drug using B3LYP/6-31G (*d*) method. Nanotube/calix[4]arenes and fluorouracil reaction are shown in Equations 1 and 2.

$$\text{Fluorouracil} + \text{Nanotube}\ (6,6) \rightarrow \text{Fluorouracil–Nanotube}\ (6,6) + \text{HF}\ (\text{bond C-C}) \quad (1)$$

$$\text{Fluorouracil} + \text{Calix[4]arene} \rightarrow \text{Fluorouracil–Calix[4]arene} + \text{HF}\ (\text{bond C-O}) \quad (2)$$

Competing interests

The authors declare that they have no competing interests.

Authors' contributions

KZ and NSH both contributed to this research work. Both authors read and approved the final manuscript.

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