Design and Measurement of novel Nanotube(6,6) and Calix[n]arene derivatives Thermodynamic Function as drug delivery by DFT

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Introduction:

Calixarenes are a group of organic macrocyclic agents that have cup like shape which are easily available through the cyclocondensation of para-substituted phenols with formaldehyde. One way to increase the aqueous solubility of drugs is to use complexing agents to form hast- guest complexes [1-2]. Single-walled carbon nanotube (SWCNTs) is allotropes of carbon with a cylindrical nanostructure. The covalent attachment of chemical group to SWCNTs is very promising for the applications of drug delivery and gas sensing properties [3, 4]. Calixarenes are promising materials for nanomedicine application in drug delivery systems. For example hydrophilic derivatives have shown interesting levels of activity against bacteria, fungi, cancerous cells and enveloped viruses, but also against thrombosis or fibrosic diseases. These applications can be obtained from Natotubes, too. Because of the safe delivery of drugs in human body, in this paper ability of Calixarenes and Nanotube in transporting skin anticancer is compared.

Computational Method:

This investigation is carried out by a pc computer which has Intel (R) Pentium (R) Dual CPU with 2GB RAM. A Nanotube (6, 6)(composit1)، Calix[6]arene(different sit, C-O, N-O; 2,3) Calix[4]arene (4) and p-sulfonato-calix[4]arene (5) including different atom number which reacts with Fluorouracil drug. The drug delivery properties are investigation. Nanotube is formed by Nanotub Modeler package [5]. The DFT Calculations have been performed using the Gauss view [6] and Gaussian 09 [7] by B3LYP method and 6-31G (d) standard basis set.

Then complex between Nanotube and derivations Calix[n]arenes with Fluorouracil drug are formed, optimized ΔG° and ΔH° by B3LYP/6-31G (d) method.

Result and discussion:

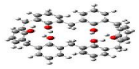
The ΔG°, ΔH°, gap energies and formation constant, $\sum E^2$ for five composites calculated with B3LYP method and 6-31G (d) basis set. For optimized and frequencies (1-5) composites were calculated. The obtained results are shown in undergo table.

Agent	ΔG°/ KJmol^{-1}	ΔH° / KJmol^{-1}	ΔE°/ KJmol-1	Formation constant (log K)	Gap of energy/ KJmol^{-1}	$\sum E^2$
Composite1	**-1.8185**	**-13.2804**	**-13.2752**	**0.3187**	**0.2923**	**47.55**
Composite2	**-141974.54**	**-141976.76**	**-141976.75**	**24869.76**	**0.6485**	**16.27**
Composite3	**-141990.62**	**-141992.92**	**-142115.78**	**24872.98**	**0.5545**	**23.53**
Composit4	**-141980.38**	**-141981.64**	**-141981.63**	**2471.01**	**0.6846**	**20.8**
Composite5	**-5.09166**	**-38.9006**	**-38.8979**	**0.8919**	**0.7874**	**53.63**

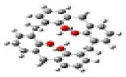
Conclusion:

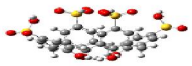
The composite (3) is more stable than other complexes. The ΔG°, ΔH°, ΔE°, in composite is more negative and it can be well reasonable for stability in it. The composite (3) are batter transport for drug delivery than other them. The different drugs delivery is shown in below.


1. Nanotube (6, 6)


2. Calix[6]arene


3.Foluoracil


4.Calix[4]arene


5.p-Sulfonatocalix[4]arene

Reference:

[1] C.D. Gutsche, "Topic in calixarene chemistry"J.Inclusion phenomena and molecular recognition in chemistry; 7, 61-72, 1989.
[2] M. Kaddouri "Novel calixarene derivatives as inhibitors of mild C-38 steel corrosion in 1 M HCl" J. Appl Electrochem 38, 1253–1258, 2008.
[3] Li. wang et al,"The synthesis of nitrogen-containing calixarene derivatives and their interactions with lead ions". J.Inclusion Phenomena and Macrocyclic Chemistry; 42, 39–43, 2002
[4] G. Pastorin" crucial functionalizations of carbon nanotubes for improved drug delivery: a valuable option?" J. Pharmaceutical Research;26,4, 2009 .
[5] www.jcrystal.com/products/wincnt/Nanotube.
[6] A. Frisch, A. B. Nielsen and A. J. Holder, Gaussview user Manual, Gaussion Inc, 2000.
[7] M. J. Frisch. etal.,Gaussian 09 , Revision D . ol, Gaussian Inc . Walling fordct, 2009

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