Theoretical Study of Doped Fullerene for Transport and Detection of Carbamazepine

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Introduction

Recently, many studies based on carbon nanostructures have led to the development of new and efficient methods for drug detection and delivery ^{1,2}. Due to its good physical-chemical sensitivity and high chemical reactivity, fullerenes and their derivatives are great candidates to be applied in this technology.³

In this work, we present the first steps adopted with the goal of studying the use of C₆₀ for both transport and detection of carbamazepine (CBZ). We present here the first results of the energy values and wavefunctions of HOMO and LUMO orbitals. It will be also presented a brief discussion of the next steps to conclude this work.

Methodology

By means Density Functional Theory (DFT), we have computed the electronic properties of doped fullerenes. The notation for doped fullerenes adopted here is X-C59 with X = Al, B, Ga, Ge, N, O, S and Si. The electronic calculations have been made using five functionals, namely: B3LYP, CAM-B3LYP, WB97X-D, PBE and LC-PBE using the 6-31G(d) basis set. All calculation it is being implemented at the Gaussian g09 software. The energy of HOMO (E_h), LUMO (E_l) orbitals and the gap between these energy values (E_g) were obtained by the equation $E_g = E_l - E_h$.

For the next step, we are performing calculation of interaction energy between the carbamazepine and fullerene molecule through the equation: E

E_{int}). Here: E_{int} represents the interaction energy between the monomers, E_{dimer} , the energy of fullerene dimer, $E_{mon,1}$ and $E_{mon,2}$ represent the monomer 1 energy and monomer 2 energy, respectively. The Basis Set Superposition Error (BSSE) has been taken care of by means of the counterpoise method.⁴

All interaction calculations are being performed taking in count the two configurations of the CBZ molecule, displayed in the next figure.

Figure 1-The two configurations which the calculation of interaction energy that are being performing.

Results

E_h , E_l and E_g energies calculated with B3LYP/6-31G(d) and WB97XD/6-31G(d) are presented below.

Figure 2-Variation of E_h , E_l and E_g for the C_{60} and X- C_{59} . Table 1- E_h , E_l and E_g energy values. The last column presents the perceptual variation (ΔE_g) of E_g with respect the C_{60} for each one of X- C_{59} .

Molecule	WB97X-D (eV)			ΔE_g %
	E_g	E_h	E_l	
CBZ	8.27069	-7.78306	0.48763	-----
C_{60}	6.04070	-7.83150	-1.79080	-----
Al- C_{59}	5.54382	-7.19475	-1.65093	-8.22554
B- C_{59}	5.72151	-7.51748	-1.79597	-5.28399
Ga- C_{59}	5.55661	-7.24999	-1.69338	-8.01381
Ge- C_{59}	5.25484	-7.62660	-2.37176	-13.0094
N- C_{59}	4.33562	-6.18465	-1.84903	-28.2265
O- C_{59}	4.87986	-6.75773	-1.87787	-19.217
S- C_{59}	5.05238	-6.84018	-1.78780	-16.361
Si- C_{59}	5.33456	-7.56265	-2.22809	-11.6897

Discussion

Through the results presented for Figure 2 and Table 1 we see that, in general, the X- C_{59} presented a decrease in the E_g with relation to the C_{60} fullerene. Among the X- C_{59} molecules, N- C_{59} showed the largest decrease in the E_g . This indicates that this derivative is chemically more reactive than the other doped molecules. For almost all doped fullerenes, it was observed a behavior electrophilic in the region around the dopant atom. The exceptions were observed for O- C_{59} , which presented an increase of electrons around the O atom and for Ge- C_{59} that apparently did not presented a significant charge exchange.

Conclusions

Looking at the perceptual variation in the ΔE_g , one can conclude that the largest variations were observed for N- C_{59} , followed by O- C_{59} and S- C_{59} . This result suggests that we can suppose that these molecules have a greater chance to adsorb, detect and deliver carbamazepine.

Our next step is to calculate the interaction energy between CBZ and X- C_{59} molecules. This will be helpful to estimate the capacity of doped fullerenes of be used as detector and as a tool to deliver carbamazepine. Spectroscopic and thermodynamics properties will also be investigated for these complexes in this work in future stages.

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