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DFT calculations of spectroscopic properties of drug delivery systems formed by oxidized carbon nanostructures

Leonardo A. De Souza[a], Diego Paschoal[b], Hélio F. Dos Santos[b], Luciano T. Costa[c], Wagner B. De Almeida[a]

[a] LQC, Departamento de Química Inorgânica; [c]MOLMOD-CS, Departamento de Físico-Química, Instituto de Química, Universidade Federal Fluminense, Campus do Valonguinho, Centro, Niterói, RJ 24020-141, Brazil.
[b]NEQC, Departamento de Química, ICE, Universidade Federal de Juiz de Fora, Campus Universitário, Martelos, Juiz de Fora, MG 36036-330, Brazil.

Abstract: Drug delivery systems (DDS) formed by oxidized carbon nanostructures are attractive systems and require specific studies of the inclusion compounds formation, interaction type, stability and spectroscopic characterization [1,2]. In the present study, DFT methods were used to study inclusion complexes formed between cisplatin and busulfan antitumor drugs (AD) with oxidized carbon nanotube (CNTox) and nanocone (CNCox) molecules (Figure 1). Gauge-Independent Atomic Orbital (GIAO) method was used for the calculation of ^{1}H and ^{195}Pt (protocol proposed by Paschoal et. al. [3] to cisplatin) magnetic shielding constants. Solvent effects on the calculation of NMR chemical shifts was evaluated using PCM and water solvent. The B3LYP/6-31G complexes geometries were used for calculations of vibrational modes of IR and Raman spectra. All calculations were performed with the Gaussian 09 package. Molecular modeling studies reported in this work can assist the experimentalists in the spectroscopic characterization of DDS formed by AD and carbon nanostructures.

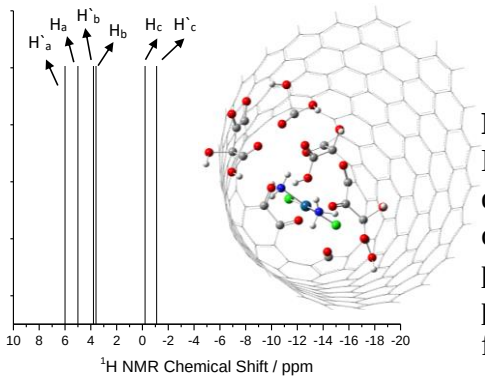

Figure 1. B3LYP/6-31G(d,p)-PCM(H_2O) ^{1}H NMR spectrum shows that the experimental detection of the inclusion complexes formed by cisplatin and oxidized carbon nanocone can be promptly attained. It was observed variations of -6 ppm due to the formation complex compared to the free cisplatin.

Key-words:DDS, Oxidized carbon nanostructures, DFT calculations, ^{1}H and ^{195}Pt RMN
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References:

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