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Editorial Open Access

Ab Initio and Density Functional Theory (DFT) Studies of Dynamic NMR Shielding Tensors and Vibrational Frequencies of DNA/RNA and Cadmium Oxide (CdO) Nanoparticles Complexes in Human Cancer Cells

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Editorial

Equilibrium constants of Cadmium Oxide (CdO) nanoparticles complexes in human cancer cells with DNA/RNA ligands have been studied with biospectroscopic methods such as ^{1}HNMR, ^{13}CNMR, ^{31}PNMR, Attenuated Total Reflectance Fourier Transform Infrared (ATR–FTIR) and FT–Raman spectroscopies in cosolvent systems at 10, 20, 30°C ± 0.5 and 1 mol.dm^{-3} ionic strength, was maintained using Sodium Chloride (NaCl) and Phosphate buffer [1-27]. The stability constants of the complexes and the resulting free–energy changes are obtained. The results are discussed in terms of effect of solvent on protonation and complexation [28-47].

The interaction between DNA/RNA and Cadmium Oxide (CdO) nanoparticles are investigated by HF, PM3, MM2, MM3, AM1, MP2, MP3, MP4, CCSD, CCSD (T), LDA, BVWN, BLYP and B3LYP methods using 31G, 6-31G*, 6-31+G*, 6-31G (3df, 3pd), 6-311G, 6-311G* and 6-311+G* basis sets of the Gaussian 09. The structural, thermodynamic, biospectroscopic and vibrational properties of DNA/RNA and Cadmium Oxide (CdO) nanoparticles complexes in human cancer cells are studied by HF, PM3, MM2, MM3, AM1, MP2, MP3, MP4, CCSD, CCSD (T), LDA, BVWN, BLYP and B3LYP methods using 31G, 6-31G*, 6-31+G*, 6-31G (3df, 3pd), 6-311G, 6-311G* and 6-311+G* basis sets of the Gaussian 09. Also, interaction energies (ΔE) were calculated. Furthermore, some of bond lengths, angles and torsions were compared. Moreover, results of rotation about two bonds were reported. In addition, Natural Bond Orbital (NBO) studies were performed to the second–order perturbation estimates of donor–acceptor interaction has been done.

The experimental ^{1}HNMR, ^{13}CNMR, ^{31}PNMR, Attenuated Total Reflectance Fourier Transform Infrared (ATR–FTIR) and FT–Raman spectra of Cadmium Oxide (CdO) nanoparticles complexes in human cancer cells with DNA/RNA ligands were recorded in $CDCl_3$ at temperature range 250–350 (K). The variable temperature spectra revealed a dynamic NMR effect which is attributed to restricted rotation around the C–C double bond. Value of 29.93 (kcal/mol) was obtained for the corresponding barrier at coalescence temperature.

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