STRUCTURAL INVESTIGATIONS ON SOME MOLECULAR COMPOUNDS OF BIOMEDICAL INTEREST

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Abstract. *Experimental FT-IR, Raman, SERS, NMR, EPR and theoretical DFT studies on pharmaceutical compounds as metoclopramide, paroxetine, amlodipine, pindolol, verapamil, metoprolol and metal complexes of Pd(II) with theophylline and Cu(II) with ^{15}N- lysine or ^{15}N-ornithine are reported. The optimized molecular structure, molecular electrostatic potential (MEP) and experimental vibrational spectra were assigned according to DFT calculations, B3LYP/6-31G(D) level of theory, in order to establish their electrophilic attack and nucleophilic reactions positions, the adsorption geometry to the silver colloidal nanoparticles and also the hydrogen bonding interactions. The elucidation of the interaction mode of metal ions with aminoacids and theophylline are significant as models for metalloproteins and also to the coordinations with major constituents of DNA and RNA. The most stable conformes, protonated and neutral forms of molecular species corresponding to a local minimum potential energy were also established.*

Keywords: biomedical compounds, spectroscopic methods, DFT calculations

Introduction

Various experimental techniques (X-ray diffraction, FT-IR, Raman, NMR, EPR) and quantum chemical calculations were shown to be very useful for structural characterization of biomedical compounds, and for a good understanding of their pharmacological activity [1–3].

Since different conformations or enantiomers of such molecules can drastically influence their physico-chemical behavior and pharmacological activity, the knowledge of their structures is of utmost importance.

From the experimental methods, Raman scattering offers important structural information making it a powerful molecular investigation tool. When the molecules are adsorbed to rough metal surfaces the Raman cross section is enhanced several orders of magnitude and analytes in the micro-molar

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