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Interaction Evaluation of Silver Ion and Silver Nanoparticles with Dithizone Complexes Using DFT Calculations and NMR Analysis

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Abstract : Silver has distinct antibacterial properties and has been used as a component of commercial products with many applications. An increasing number of commercial products cause risks of silver effects for human and environment such as the symptoms of Argyria and the release of silver to the environment. Therefore, the detection of silver in the aquatic environment is important. The colorimetric chemosensor is designed by the basic of ligand interactions with a metal ion, leading to the change of signals for the naked-eyes which are very useful method to this application. Dithizone ligand is considered as one of the effective chelating reagents for metal ions due to its high selectivity and sensitivity of a photochromic reaction for silver as well as the linear backbone of dithizone affords the rotation of various isomeric forms. The present study is focused on the conformation and interaction of silver ion and silver nanoparticles (AgNPs) with dithizone using density functional theory (DFT). The interaction parameters were determined in term of binding energy of complexes and the geometry optimization, frequency of the structures and calculation of binding energies using density functional approaches B3LYP and the 6-31G(d,p) basis set. Moreover, the interaction of silver–dithizone complexes was supported by UV–Vis spectroscopy, FT-IR spectrum that was simulated by using B3LYP/6-31G(d,p) and 1H NMR spectra calculation using B3LYP/6-311+G(2d,p) method compared with the experimental data. The results showed the ion exchange interaction between hydrogen of dithizone and silver atom, with minimized binding energies of silver–dithizone interaction. However, the result of AgNPs in the form of complexes with dithizone. Moreover, the AgNPs-dithizone complexes were confirmed by using transmission electron microscope (TEM). Therefore, the results can be the useful information for determination of complex interaction using the analysis of computer simulations.

Keywords : silver nanoparticles, dithizone, DFT, NMR
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