Potentiometric Study, DFT Calculations and Thermodynamic Parameters of Complex Formation between Cd(II) and Thiosemicarbazone Ligand

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(E)-N-methyl-2-((E)-1-(2-(p-tolyl)hydrazono)propan-2-ylidene)hydrazine-1-carbothioamide (MTHPH) has been synthesized and characterized using elemental analyses, IR, mass spectra and ¹H-NMR measurements. The antibacterial, antifungal and antioxidant activity studies of the synthesized MTHPH ligand was investigated and discussed. Molecular modeling was drawn for MTHPH thiosemicarbazone compound and its molecular parameters were determined. Novel MTHPH ligand protonation constants and its formation constants with Cd(II) ion were determined in 50% DMSO solution at 15 °C, 25 °C and 35 °C. The solution speciation of different species was measured as a function of pH. Calculation and discussion of the thermodynamic parameters were accomplished. Both log K₁ and –ΔH₁, for Cd(II)-complexes have been observed to some degree greater than log K₂ and –ΔH₂, indicating a change in the dentate character of this ligand from tridentate donors in 1:1 chelates to bidentate in 1:2; M:L chelates in addition to steric hindrance induced by entry of 2nd molecule. MTHPH compound may be considered as a good remedy for Cd²⁺ toxicity.

Keywords: Potentiometry; Schiff base; thermodynamics, speciation, Mass spectra, Cadmium.

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