Potentiometric Study of a New Schiff Base and its Metal Ion Complexes: Preparation, Characterization and Biological Activity

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Some metal complexes of a new Schiff base [4-(morpholin-4-yl)benzylidenyl]thiosemicarbazide (L) have been investigated. A potentiometric method was used to determine their stability constants by pH-metric titration. The stoichiometric protonation constants of L in 25 % (v/v) ethanol-water mixture and ionic strength of 1 mol dm⁻³ were found to be 4.88 and 10.21. The formation constants of the complexes increase in the order of La(III) > Fe(III) > Co(II) > Cu(II) > Mn(II) > Pd(II) > Ni(II) ions. The chemical structure of L and its metal complexes were established using elemental analyses and infrared spectroscopy. The microanalytical data reveals that a 1:1 (metal:ligand) stoichiometric ratio was found for the compounds. The geometric parameters of the metal-L complexes were assumed according to the density functional theory (DFT) method. The complexes show a moderate antibacterial inhibition against *Staphylococcus aureus* and *Escherichia coli* and a fair degree of antifungal activity against *Aspergillus fumigatus*, *Alternaria alternata* and *Fusarium oxysporum*.

Keywords: Potentiometric, new Schiff base, metal complexes, theoretical studies, antimicrobial activity.

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