Fayoum University

Faculty of Science

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"SYNTHESIS, SPECTROSCOPIC CHARACTERIZATION, THEORETICAL STUDIES, BIOLOGICAL AND CATALYTIC APPLICATIONS OF SOME SCHIFF BASES TRANSITION METAL COMPLEXES"

By

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ABSTRACT

"Synthesis, Spectroscopic Characterization, Theoretical Studies, Biological and Catalytic Applications of Some Schiff Bases Transition Metal Complexes"

Schiff bases have a great interest for their important properties, such as their catalytic activity in the hydrogenation of olefins, ability to reversibly bind oxygen in epoxidation reactions, photochromic properties and complexing ability towards some toxic metals. Moreover, Schiff base complexes displayed an important role in biological activity applications. Many investigations have been widely studied on metal complexes of Schiff bases containing N and/or O donor sites, while fewer studies were performed for those having ONS donor atoms.

Thereaction ofCo(II), Ni(II), Cu(II), Zn(II), Cd(II), Hg(II), Pt(II), Pd(II),$Mo(CO)_6$and $Ru_3(CO)_{12}$ with the synthesized N-(2-hydroxy-1-naphthylidene)-2-aminothiophenol Schiff base ligand (H_2L1) resulted in the formation of the ten complexes; $[Co(HL1)_2]H_2O$;**1,**$[Ni(HL1)_2]$;**2,** $[M(HL1)_2]$ (M= Cu, Zn and Cd); **(3-5)** and [Hg(HL1)Cl];**6,[**$Pd_2(HL1)_2Cl_2$];**7, [**$Pt(H_2L1)Cl_2$];**8,**$Mo(O_2)(H_2L1)$;**9,**$[Ru(CO)_3(HL1)]$;**10**. The ligand and its complexes were characterizedbased on elemental analyses, IR, ^{1}H NMR, mass spectrometry, magnetic measurement, molar conductance, and thermal analysis.Coats and Redfern method was used to compute the kinetic and thermodynamic parameters. Antibacterial activities of $H_2L1$and its complexes have been studied. The binding of the reported complexes to calf thymus DNA (CT-DNA) has been investigated using UV-Vis and fluorescence absorption spectra. The results indicated that the ligand and its complexes may bind to DNA by intercalation modes, with a much higher binding affinity of the complexes than that of the ligand.The equilibrium geometries of the studied complexes were investigated theoretically at the B3LYP/LANL2DZ level of theory, and it was found that these geometries are non- linear. The calculated E_{HOMO} and E_{LUMO} energies of the studied complexes can be used to calculate the global properties. The calculated nonlinear optical parameters (NLO); first order hyperpolarizibility (β) of the studied complexes showed promising optical properties.

Furthermore, Thiophene-Iminopyridyl Schiff bases and their palladium complexes were synthesized and characterized by the spectroscopic techniques including x-ray crystallography and NOESY NMR spectroscopy. These potential palladium-Schiff base complexes were checked for Heck-Coupling reaction and they showed high catalytic activity in this reaction.

Moreover, N5 pentadentate ligand and its Co(II) and Ni(II) complexes were synthesized, spectroscopic characterized and investigated in catalytic activity for water oxidation. Cobalt complex displayed more catalytic activity than nickel complex.