

Synthesis, Characterization, DFT Calculations, NLO Properties and Different Applications of Ni(II), Pd(II), Pt(II), Mo(IV) and Ru(I) Complexes with NOS Schiff Base

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Thermal reaction of $\text{Ni}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$, PdCl_2 , PtCl_2 , $\text{Mo}(\text{CO})_6$ and $\text{Ru}_3(\text{CO})_{12}$ with the prepared Schiff base ligand N-(2-hydroxy-1-naphthylidene)-2-aminothiophenol (H_2L) resulted in the formation of the five complexes; $[\text{Ni}(\text{HL})_2]$, **1**; $[\text{Pt}(\text{H}_2\text{L})\text{Cl}_2]$, **2**; $[\text{Pd}_2(\text{HL})_2\text{Cl}_2]$, **3**; $[\text{Mo}(\text{O}_2)(\text{H}_2\text{L})]$, **4**; and $[\text{Ru}(\text{CO})_3(\text{HL})]$, **5**. The studied compounds were characterized using different spectroscopic techniques (IR, ^1H NMR, mass) elemental analyses, magnetic measurement, molar conductance, and thermal analysis. Theoretical calculations based on accurate DFT approximations were used to verify the structures of ligand and complexes. Coats and Redfern method was used to compute the kinetic and thermodynamic parameters. The relative reactivities were estimated using chemical descriptors analysis. The antioxidant activity against DPPH radical was evaluated *in vitro* by using spectrophotometric methods; the experiments showed potent antioxidant activity. Also, the interaction of the reported compounds with calf thymus DNA (CT-DNA) by different techniques revealed that the complexes could bind to CT-DNA by intercalative mode. Antibacterial activities of the synthesized compounds have been studied against Gram-positive and Gram-negative bacteria by the agar well diffusion. The antifungal activity of the synthesized compounds was tested using agar well diffusion method. The binding of the reported complexes to calf thymus DNA has been investigated using fluorescence and UV-Vis absorption spectra. The results indicated a much lower binding affinity of the ligand than that of the complexes.

Biography:

Dr. Samir Moustafa El-Medani is a Professor of Inorganic Chemistry, Department of Chemistry, from Fayoum University, Egypt. He did Bachelor of Science Degree, Department of Chemistry, Cairo University, 1967 & M. Sc. Degree in Analytical Chemistry, Ain Shams University, 1977 and Ph.D. of Science in Inorganic Chemistry, Ain Shams University, 1985.

He was a Lecturer of Chemistry Department Sana'a University, Assistant Professor, Chemistry Department from Cairo University, Fayoum Branch, 1993.

He is a Chief of research team concerning a project entitled "Spectroscopic Studies on the complexes resulting from the interaction of carbonyls with some transition elements pyridine derivatives" K.S.A., Umm Al-Qura University, K.S.A. And the main supervisor for several Theses in Inorganic and Analytical Chemistry, have 60 international researches & Participation in the several International Conferences.