

(البحث رقم 9 في القائمة الرئيسية)

Synthesis, characterization, NLO properties, antimicrobial, CT-DNA binding and DFT modeling of Ni(II), Pd(II), Pt(II), Mo(IV) and Ru(I) complexes with NOS Schiff base		عنوان البحث : (باللغة الإنجليزية)
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ملخص موجز للبحث :

The 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 previously prepared Schiff base ligand N-(2-hydroxy-1-naphthylidene)-2-aminothiophenol (H_2L) resulted in the formation of the following 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 various spectroscopic techniques (IR, ^1H NMR, mass spectrometry), elemental analysis, magnetometry, molar conductivity and thermal analysis. The kinetic and thermodynamic parameters of the complexes were calculated. The geometries of the studied 1:1 Pt(II)-, Pd(II)-, Mo(IV)-, and Ru(I)-complexes and the 1:2 Ni(II)-complex were investigated based on the B3LYP/GENECP level of theory. The geometries of the studied complexes are non-planar as evidenced by the dihedral angle between the central metal ion and the coordinating ligand atoms. DFT calculations were also performed to calculate the general properties; hardness (η), global ductility (S), and electronegativity (χ). The average first-order hyperpolarization ($\langle\beta\rangle$) was calculated and compared with urea as a reference material. The first-order hyperpolarization ($\langle\beta\rangle$) results demonstrated that the ligands and the studied complexes are excellent candidates for NLO materials. The interaction of the complexes with calf thymus DNA (CT-DNA) using various techniques also showed that the complexes can bind to CT-DNA via an interfering mode. The binding of the aforementioned complexes to calf thymus DNA was studied using fluorescence, UV-vis absorption spectra, and fluorescence spectra. The results indicated that the binding capacity of the ligands was significantly lower than that of the complexes. The biological activities of the compounds were also studied.

