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Synthesis, Spectral Characterization, Thermal and Theoretical Studies of Two Co(II) and Ni(II) Coordination Complex with N, O Donor of 2-Chloro-6-[(3-hydroxy-4-methoxybenzylidene) amino]-4-Nitrophenol

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ABSTRACT

We report here two mononuclear Co(II) and Ni(II) complexes of general formula $[M(L)_2(H_2O)_2].xH_2O$, {M:Co^{II} and Ni^{II}; x:2} derived from 2-chloro-6-[(3-hydroxy-4-methoxybenzylidene) amino]-4-nitrophenol ligand. Synthesized compounds were characterized by elemental analysis, FT-IR, UV-Visible, molar conductance, thermal, PXRD and SEM. Distorted octahedral geometry was suggested for both complexes around the metal center with ligand. The Powder X-ray diffraction pattern and SEM analysis shows the crystalline nature of complexes. Thermal studies of the synthesized complexes show their general decomposition pattern and thermal stability. The kinetic and thermodynamic parameters viz. activation energy (E^*), entropy of activation (ΔS^*), enthalpy of activation (ΔH^*) and free energy of activation (ΔG^*) of degradation process were also evaluated using Coats-Redfern (C-R) and Horowitz–Metzger (H-M) methods for both complexes assuming first order degradation. In addition theoretical calculations by means of DFT at B3LYP level were incorporated to support the experimental findings.

Graphical Abstract

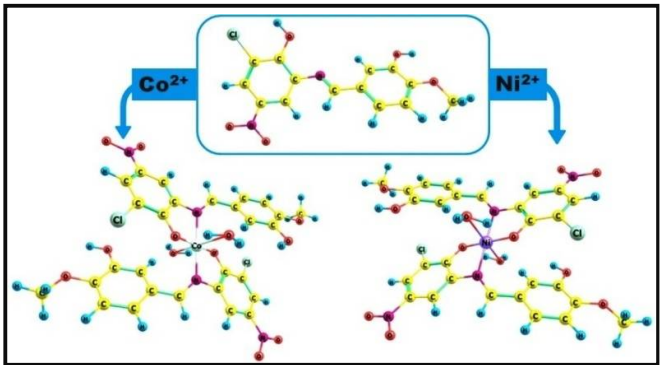

Figure 7. DFT optimized Structure of ligand (HL) using B3LYP/6-31G basis set and its Co (II)- and Ni(II)-complex using B3LYP/LANL2DZ basis set.

Keywords: Schiff base-metal complexes, Thermal studies, Electrochemical studies, XRD, DFT.