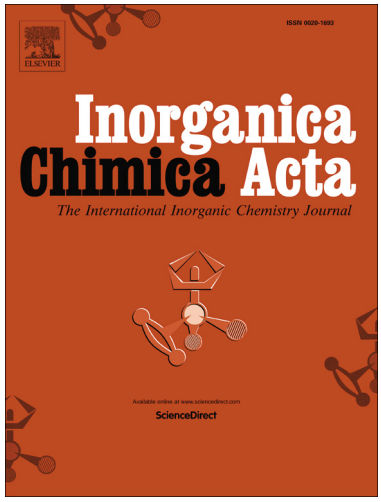

Research paper

Synthesis, crystal structure, electrochemical properties and DFT calculations of three new Zn(II), Ni(II) and Co(III) complexes based on 5-bromo-2-((allylimino)methyl)phenol Schiff-based ligand

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Synthesis, crystal structure, electrochemical properties and DFT calculations of three new Zn(II), Ni(II) and Co(III) complexes based on 5-bromo-2-((allylimino)methyl)phenol Schiff-based ligand

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Abstract:

In this work, a new Schiff base ligand (HL: 5-bromo-2-((allylimino)methyl)phenol) was prepared from the reaction of 5-bromo salicylaldehyde and allylamine. Then, three new Schiff base complexes, ZnL_2 **(1),** NiL_2 **(2)** and CoL_3 **(3)**, were synthesized through the reaction of $Zn(NO_3)_2.6H_2O$, $Ni(OAC)_2{\cdot}4H_2O$, and $CoCl_2.6H_2O$ with the new Schiff base ligand in methanol or chloroform. The ligand and its related complexes were characterized by elemental analysis, FT-IR, UV-Vis spectroscopy, and ^{1}H- NMR technique. The molecular structures of complexes **(1-3)** were determined by the single crystal X-ray diffraction technique. The crystallographic data revealed that complexes **1** and **2** are four-coordinated by two phenolate oxygen and two imine nitrogen atoms of two Schiff base ligands. On the other hand, the metal center is six-coordinated by three phenolate oxygen and three imine nitrogen atoms of three Schiff base ligands in **3**. Eventually, DFT calculations and the study of electrochemical properties were performed on the new three complexes.

Keywords: Schiff base, Crystal structure, Electrochemical properties, DFT studies.

1. Introduction