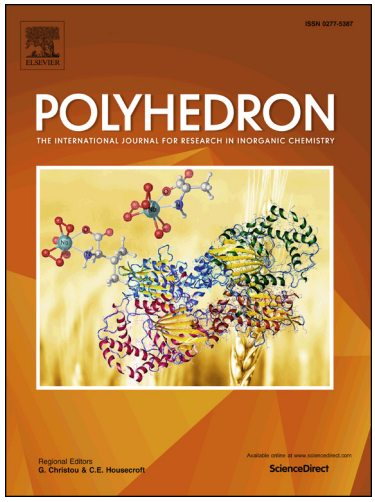

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X-ray diffraction, spectroscopic and DFT studies on Nickel(II)-triphenylphosphine complexes of 2-hydroxyacetophenone thiosemicarbazones

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Abstract

This work presents a combined experimental and theoretical study on new synthesized *ONN* and *ONS* chelatig 2-hydroxyacetophenone thiosemicarbazone ligands and their nickel(II) complexes with triphenylphosphine co-ligand. The 5-bromo-2-hydroxyacetophenone thiosemicarbazone ligand (**L^1**) coordinates to nickel through the phenolic-O, azomethine-N and thiole-S atoms and the complex [Ni(L^1)(PPh$_3$)] (**1**) is formed an *ONSP* donor set with P atom of triphenylphosphine ligand. The 5-bromo-2-hydroxyacetophenone-*S*-methyl-thiosemicarbazone ligand (**L^2**) is functional a thioamide nitrogen instead of a sulfur atom, so complex [Ni(L^2)(PPh$_3$)] (**2**) have *ONNP* donor set. The spectroscopic properties of all compounds have been determined by IR, ^{1}H NMR and UV-Vis spectroscopy techniques and the crystal structure of **L^1**, **1** and **2** have also been studied using X-ray diffraction. The molecular geometries obtained by X-ray analyzes in the ground state were compared with the optimized geometries which were calculated using the DFT/B3LYP method. The 6-311G(d,p) basis set for C, H, N, O, P, S atoms and LANL2DZ basis set for Ni atom were chosen in all theoretical calculations. In addition to molecular geometries, the vibrational frequencies, electronic transitions and ^{1}H NMR chemical shifts of the compounds were computed and compared with the experimental values. The electronic absorption spectra of the both complexes were predicted by using the time-dependent DFT method. The HOMO-