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Işın Kılıç-Cıkla, Şükriye Güveli, Tülay Bal-Demirci, Muhittin Aygün, Bahri Ülküseven, Metin Yavuz

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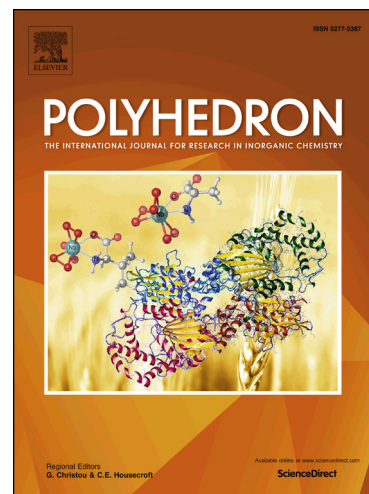
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# X-ray diffraction, spectroscopic and DFT studies on Nickel(II)- triphenylphosphine complexes of 2-hydroxyacetophenone thiosemicarbazones

Işın Kılıç-Cıkla<sup>a,\*</sup>, Şükriye Güveli<sup>b</sup>, Tülay Bal-Demirci<sup>b</sup>, Muhittin Aygün<sup>c</sup>,  
Bahri Ülküseven<sup>b</sup>, Metin Yavuz<sup>a</sup>

<sup>a</sup>Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, 55139, Samsun,  
Turkey

<sup>b</sup>Department of Chemistry, Engineering Faculty, Istanbul University, 34320, İstanbul, Turkey

<sup>c</sup>Department of Physics, Faculty of Arts and Sciences, Dokuz Eylül University, 35160, İzmir, Turkey

## Abstract

This work presents a combined experimental and theoretical study on new synthesized *ONN* and *ONS* chelating 2-hydroxyacetophenone thiosemicarbazone ligands and their nickel(II) complexes with triphenylphosphine co-ligand. The 5-bromo-2-hydroxyacetophenone thiosemicarbazone ligand (**L**<sup>1</sup>) coordinates to nickel through the phenolic-O, azomethine-N and thiole-S atoms and the complex [Ni(L<sup>1</sup>)(PPh<sub>3</sub>)] (**1**) is formed an *ONSP* donor set with P atom of triphenylphosphine ligand. The 5-bromo-2-hydroxyacetophenone-S-methyl-thiosemicarbazone ligand (**L**<sup>2</sup>) is functional a thioamide nitrogen instead of a sulfur atom, so complex [Ni(L<sup>2</sup>)(PPh<sub>3</sub>)] (**2**) have *ONNP* donor set. The spectroscopic properties of all compounds have been determined by IR, <sup>1</sup>H NMR and UV-Vis spectroscopy techniques and the crystal structure of **L**<sup>1</sup>, **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 <sup>1</sup>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-

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