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# Synthesis, structural characterization, DFT studies and biological activity of Cu(II) and Ni(II) complexes of novel hydrazone

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## Abstract

Novel hydrazone 2-(2-((1*E*,2*E*)-2-(2-phenylhydrazineylidene)propylidene)hydrazineyl)pyridine and its nickel(II) and copper(II) complexes have been synthesized and characterized. The ligand (H<sub>2</sub>PGI) was prepared by the condensation reaction of 1-(2-phenylhydrazineylidene)propan-2-one and 2-hydrazinopyridine. The crystal structure of Ni(II) complex was determined. In both Ni(II) and Cu(II) complexes, H<sub>2</sub>PGI act as a neutral tridentate ligand forming two fused five-membered chelation rings through NNN set of donor atoms. Octahedral geometry is proposed for both chelates as illustrated in both magnetic and spectroscopic data. ESR spectroscopy was performed for Cu(II) complex which exhibited a considerable Cu–Cu interaction and harmonize directly with measured magnetic moment. The molecular modeling structures were optimized and showed the bond length, bond angle, reactivity, MEP and atomic charges for all the title frameworks. Hypothetical infrared intensities and <sup>1</sup>H NMR of H<sub>2</sub>PGI was estimated on the basis of DFT scheme. A comparison of the experimental and theoretical data was very useful in creating correct assignments and understanding the basic chemical shift. Biological activity of the synthesized compounds were investigated versus some Gram positive, Gram negative bacteria and some fungal strains. Also, the antitumor activity was investigated.

**Keywords:** Hydrazone, biological activity, X-ray, DFT, theoretical IR

## 1. Introduction

Hydrazones and their metal complexes are the most broadly examined compounds on account of their biological behavior as anti-bacterial, antifungal and as anti-cancer agents [1-4] besides their manufacturing and pharmaceutical behavior [5]. They also exhibited redox activities, sensing probes, magnetism, supramolecular order, luminescence, optoelectric

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