



Available online at: <http://www.basra-science-journal.org>



ISSN -1817 -2695

Received 18.11.2015, Accepted 27.3.2016

## Synthesis and Study of Some Structural Properties for New Complexes derived from $\alpha$ -(phenyl)-N-phenyl nitronne with Cu(II), Co(II) and Ni (II) and Study of Their Anti-Bacterial Activity

Zainb A. Mohammed Saleh\*, Kawkab A. Hussain, Sadiq M-H. Ismael

Department of Chemistry , College of Education Pure Science , University of Basrah  
Basrah – Iraq.

[Zainab\\_alhhasb71@yahoo.com](mailto:Zainab_alhhasb71@yahoo.com)

### Abstract:

A new series of transition metal complexes of Cu (II), Co (II) and Ni (II) has been synthesized from the  $\alpha$ -(phenyl)-N-phenyl nitronne derived from N-phenyl hydroxyl amine and benzaldehyde. Their structures were elucidated using spectroscopic techniques, elemental analyses and molar conductivity. The IR and UV-Vis spectral data of the complexes suggest square planer geometry for all complexes. The theoretical calculations of nitronne complexes were studied by quantum chemical calculations. The optimized structures of the nitronne complexes were obtained by DFT/B3LYP level of theory using the basis set 6-311+G(d) for ligand and LANL2DZ for the complexes. The dipole moment of co-complex found to have high values compared with the complexes and ligand. Global descriptors such as the MO energies of HOMO, LUMO levels,  $\Delta E$  and hardness ( $\eta$ ) were determined and used to identify the differences in the stability and reactivity of compounds. In general the calculated the values lead to favorable state for stabilities (high chemical reactivity and low kinetic stability) (Li>Co >Ni>Cu). In addition the calculations show the effect of coordination and this leads to the change of the bond length and angles. The biological activity shows that the Cu (II) complex was sensitive to *S. aureus* and Co (II) complex was sensitive to *E. coli*.

**Key Words:** Nitronne complexes, Spectrophotometric, Conductivity, Antibacterial Activity, DFT/B3LYB.