

## Coordination Behavior, Theoretical studies and Biological Activity of Some Transition Metal Complexes with Oxime Ligands

**Authors :** Noura Kichou, Manel Tafergguenit, Nabila Ghechtouli, Zakia Hank

**Abstract :** The aim of this work is to synthesize, characterize and evaluate the biological activity of two Ligands: glyoxime and dimethylglyoxime, and their metal Ni(II) chelates. The newly chelates were characterized by elemental analysis, IR, EPR, nuclear magnetic resonances ( $^1\text{H}$  and  $^{13}\text{C}$ ), and biological activity. The antibacterial and antifungal activities of the ligands and its metal complexes were screened against bacterial species (*Staphylococcus aureus*, *Bacillus subtilis*, and *Escherichia coli*) and fungi (*Candida albicans*). Ampicillin and amphotericin were used as references for antibacterial and antifungal studies. The activity data show that the metal complexes have a promising biological activity comparable with parent free ligand against bacterial and fungal species. A structural, energetic, and electronic theoretical study was carried out using the DFT method, with the functional B3LYP and the gaussian program 09. A complete optimization of geometries was made, followed by a calculation of the frequencies of the normal modes of vibration. The UV spectrum was also interpreted. The theoretical results were compared with the experimental data.

**Keywords :** glyoxime, dimethylglyoxime, nickel, antibacterial activity

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