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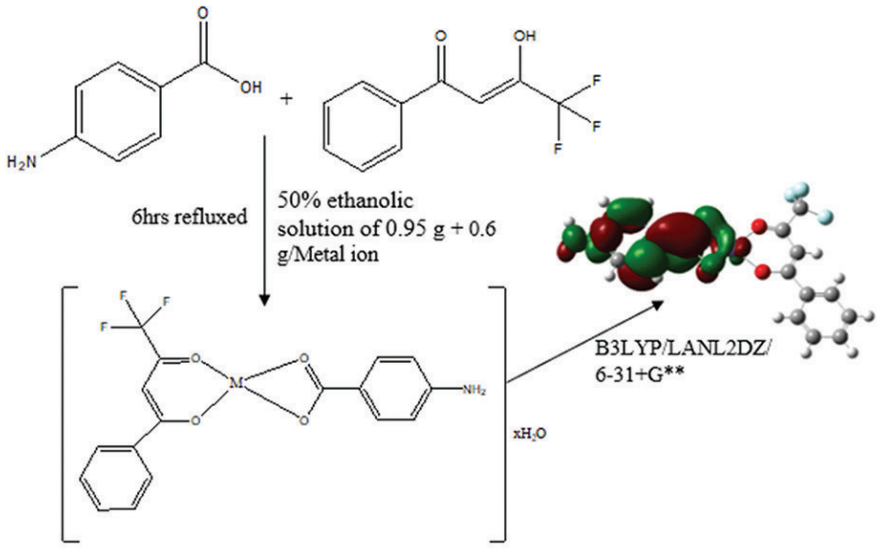
Synthesis, Characterization, and Computational Studies of Metal(II) Complexes Derived from β-diketone and Para-aminobenzoic Acid

Adesoji A. Olanrewaju[1], Collins U. Ibeji[2,3]*, Festus S. Fabiyi[1]

[1]Department of Chemistry and Industrial Chemistry, Bowen University, Iwo, Nigeria
[2]Department of Pure and Industrial Chemistry, University of Nigeria, Nsukka, Nigeria
[3]Catalysis and Peptide Research Unit, School of Health Sciences, University of KwaZulu-Natal, Durban 4041, South Africa

ABSTRACT Some metal(II) mixed-ligand complexes of Mn, Fe, Co, Ni, Cu, and Zn, derived from 4,4,4-trifluoro-1-phenyl-1,3-butanedione (Tf) and para-aminobenzoic acid (Pa) were synthesized. Spectroscopic characterization was carried which includes infrared (IR) and electronic spectra (solid reflectance) measurements. Melting points, magnetic moments at room temperature, solubility, conductivity and percentage metal were also determined. The infrared spectra measurements suggest that the metal atoms coordinated to both ligands, Tf and Pa through the O_4 chromophores. The magnetic moments, percentage metal analysis, and electronic spectra measurements were used to confirm the octahedral geometry of Co(II), Ni(II) and the four-coordinate (tetrahedral/square-planar) complexes (Mn(II), Fe(II), and Cu(II)). The non-electrolytic nature of all the synthesized complexes was shown by conductivity measurements. The density functional theory calculations for all the metal complexes also support experimental results. Mn(II) and Fe(II) complexes had lower energy gaps, indicating higher reactivity compared to others.



KEYWORDS Metal-complexes, Density functional theory, Magnetic moments, Non-electrolyte, Electronic spectra.

*Corresponding author: Email: ugochukwu.ibeji@unn.edu.ng

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