



## Full Length Article

Spectroscopic characterization, DFT calculations, *in vitro* pharmacological potentials, and molecular docking studies of *N, N, O*-Schiff base and its trivalent metal complexesIkechukwu P. Ejidike<sup>a,b,c,\*</sup>, Amani Direm<sup>d,e</sup>, Cemal Parlak<sup>f</sup>, Adebayo A. Adeniyi<sup>g,h</sup>, Mohammad Azam<sup>i</sup>, Athar Ata<sup>b,j,\*\*</sup>, Michael O. Eze<sup>b</sup>, Joshua W. Hollett<sup>b</sup>, Hadley S. Clayton<sup>a</sup><sup>a</sup> Department of Chemistry, College of Science, Engineering and Technology, University of South Africa, Florida 1710, South Africa<sup>b</sup> Department of Chemistry, Faculty of Science, The University of Winnipeg, Winnipeg, MB R3B 2E9, Canada<sup>c</sup> Department of Chemical Sciences, Faculty of Natural, Applied and Health Sciences, Anchor University, Lagos 100278, Nigeria<sup>d</sup> Laboratory of Structures, Properties and Interatomic Interactions LASPI2A, Faculty of Sciences and Technology, Abbes Laghrour University, Khenchela 40.000, Algeria<sup>e</sup> Department of Matter Sciences, Faculty of Sciences and Technology, Abbes Laghrour University, Khenchela 40.000, Algeria<sup>f</sup> Department of Physics, Faculty of Science, Ege University, Izmir 35040, Turkey<sup>g</sup> Department of Chemistry, University of the Free State, PO Box 339, Bloemfontein 9300, South Africa<sup>h</sup> Department of Industrial Chemistry, Faculty of Sciences, Federal University, Oye-Ekiti 371104, Nigeria<sup>i</sup> Department of Chemistry, College of Science, King Saud University, Riyadh 11451, Saudi Arabia<sup>j</sup> Department of Chemistry, College of Sciences and Arts, Michigan Technological University, Houghton, MI 49931, USA

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## ABSTRACT

In this study, trivalent metal complexes of the category:  $[M(L)(H_2O)_nCl_y]$  obtained from the interaction of metal<sup>3+</sup> ion salts with organic *N, N, O*-Schiff base (**HL**) (where: **HL** = 4- $\{(Z)-((2-((E)-((2\text{-hydroxyphenyl})\text{methylidene})\text{amino})\text{ethyl})\text{imino})\text{methyl})-2\text{-methoxyphenol}$ ;  $n, y = 1$  or  $2$  and  $M = \text{Ti(III), Fe(III), Ru(III), Cr(III)}$  and  $\text{Al(III)}$ ) were synthesized and characterized *via* molar conductance, FT-IR, and UV-Vis spectroscopies, elemental analyses, thermal analyses (TGA and DTA), and UV-Vis spectroscopy, theoretical calculations. A distorted octahedral structure around the metal ions was proposed based on the obtained experimental and calculated data. Thermal examination of the complexes signposts the step-by-step disintegration to give the final decomposition product as metal oxides. Moreover, DFT calculations were executed utilizing the B3LYP/LANL2DZ theory level, which revealed that the synthesized metal (III) complexes were more stable than the free ligand (**HL**). The value of  $\Delta E$  for **HL** is 4.60 eV while the related values for the complexes of Cr(III) (**C1**), Ru(III) (**C2**), Fe(III) (**C3**), Al(III) (**C4**), and Ti(III) (**C5**) are respectively 2.59, 3.68, 3.15, 1.64, and 2.75 eV. Scavenging abilities of DPPH and ABTS radicals by the test compounds revealed promising antioxidant behavior. It was observed that the compounds are proficient DPPH radical scavengers in a dose-dependent configuration. Ru(III);  $IC_{50} = 1.69 \pm 2.68 \mu\text{M}$  for DPPH and Ti(III);  $IC_{50} = 8.70 \pm 2.78 \mu\text{M}$  for ABTS performed best. Similarly, the complexes demonstrated higher antimicrobial activities compared to **HL** against the designated strains, while ciprofloxacin acted as a standard antibiotic. Furthermore, the ligand and its most effective complexes **C2** and **C5** were docked against the targets *S. aureus* DNA gyrase (**2XCT**), *S. pneumoniae* DNA gyrase (**5BOD**), and *E. coli* DNA gyrase (**5L3J**). The binding sites were evaluated and the docking results showed that the studied molecules bind to the targets through classical O—H...O and/or N—H...O hydrogen bonds, as well as *via* hydrophobic contacts.

## 1. Introduction

Schiff bases are a significant set of organic compounds specially

studied owing to their various applications [1]. Tridentate donor ligands formed by heterocyclic Schiff bases have displayed some metal complexes stabilization character, having the coordination to occur *via* the

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