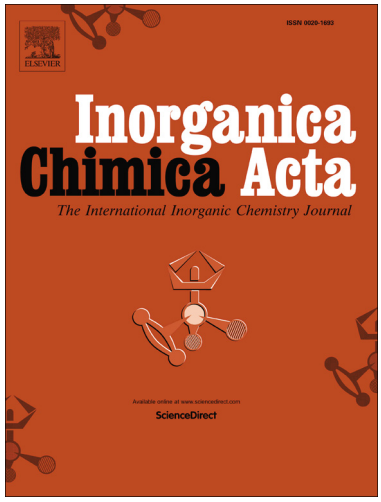

Research paper

Urinary Tract Infection Fighting Potential of Newly Synthesized Ruthenium Carbonyl Complex of N-dehydroacetic acid- N´-o-vanillin-ethylenediamine

J.M. Mir, N. Jain, B.A. Malik, R. Chourasia, P.K. Vishwakarma, D.K. Rajak, R.C. Maurya

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A B S T R A C T

In recent years, there has been a growing fascination towards the development of new antimicrobial agents from various sources to combat microbial resistance. *Kleblseilla pneumonia* and *E. coli* are the main urinary tract infection (UTI) causing agents. Herein, we report the synthesis and characterization of a novel carbonyl complex of Ru(II) that has been found a good antimicrobial agent against the selected microbes. Hence, may be suggested as potent agent against UTI. The compound on characterization was found octahedral in structure on the basis of comparative DFT-experimental characterization. Molecular specification under B3LYP functional, LANL2DZ basis set for Ru atom and 6-31g(d,p) for all other atoms were employed. Electron density plots and geometrical optimization were the main theoretical aspects that were invoked. Elemental analysis, mass spectrometry, NMR, FT-IR, UV-Vis and cyclic voltammetry were the physio-chemical techniques at both the experimental and theoretical fronts that helped to establish the proposed structure. From the overall study, it may be remarked that both observed and computed outcomes have been found in good agreement with each other.

Keywords: DFT; Ru; UTI; Carbonyl

Introduction

Biological relevance of ruthenium carbonyl complexes has attracted scientists to verify its DNA binding and anti-carcinogenic potential [1]. Complexes bearing Ru metallic core have shown excellent redox properties [2]. The investigated role of general co-ligands like hydride, carbonyl, chloride, and triphenylphosphine of this class of catalysts explored through density functional theory (DFT) have suggested some key measures involved in their reactivity. Hence may be used as a precursor for the synthesis of the new monophosphine carbonyl ruthenium coordination compounds [3]. The metal–metal linking beahiour upon protonation [4], catalytic activities of olefin metathesis [5] and other important evidences suggest ruthenium compounds to be efficient catalysts [6].