INORGANIC AND NANO-METAL CHEMISTRY
2023, VOL. 53, NO. 6, 570–578
https://doi.org/10.1080/24701556.2023.2165679

Synthesis and DFT supported spectroscopic characterization of a pyrazolone Schiff base complex of Ru^{II}-NO core

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ABSTRACT

Due to the fact of fascinating properties of 4-aminoantipyrene and other pyrazolone derivatives, this work is mainly focused on the synthesis of Schiff base complex of Ru-NO core containing pyrazolone as the main ligand functionality. Several spectroscopic and spectrometric techniques in association with theoretical approach (DFT) have been applied to elucidate the structure of the complex. In addition to the characterization, parameters that decide to label the given compound as a significant nitric oxide releasing molecule (NORM) have been discussed. DFT based computational studies using LANL2DZ/B3LYP and 6-31 G(d,p)/B3LYP formalism, respectively for Ru and non-metallic atoms of the complex have been used to deal with the NO-releasing phenomenon. From the results discussed herein it is evident that the complex can release NO at the cost of low energy radiation.

ARTICLE HISTORY
Received 17 July 2021
Accepted 29 December 2022

KEYWORDS
Ru-NO; DFT; excitation; singlet; triplet; thermal

Introduction

Medicinal inorganic chemistry is a discipline of growing significance in both therapeutic as well as diagnostic fields.[1] The chemotherapeutic agents like cisplatin and carboplatin are the prominent representatives of medicinal inorganic chemistry.[2] The field now encompasses active metal complexes, metal ions, and even metal binding compounds as potential agents.[3] Meanwhile, biological properties of ligands have been shown to enhance on metal complexation.[4] The selection of complexing ligand and the nature of a metallic core show profound implications on such applications involving antimicrobial, anticancer and several other biological aspects.[5–8] Schiff base ligands and their complexes are special class of compounds bearing a wide range applications in numerous fields of applied interest.[9–12] Over the last few decades, various metal Schiff base complexes have been widely utilized for a broad range of catalytic asymmetric reactions.[13,14] In general, azomethine metal complexes containing nitrosyl functionality are referred as interesting scaffolds of huge medicinal, environmental and industrial significance.[15–17] Similarly, Ru-nitrosyl/carbonyl complexes also represent fascinating molecular systems possessing diversified applications of scientific interest.[18,19] The biomedicinal aspects, photosensitivity and other catalytic properties shown by such compounds have been given considerable attention by the scientific community.[20,21]

The selection of ligand for complexation is an important and careful job for synthesizing a complex. Pyrazolone based Schiff base as ONO donor ligand is the second co-ligand after NO targeted in this study. Such types of cyclic ligands have been found significant in various aspects. It has been revealed that pyrazole containing pharmacoactive agents play important role in medicinal chemistry.[15, 19] Pyrazolone derivatives are counted among typical ICT (Intramolecular Charge Transfer) compounds having well pronounced transport tendency.[18] The derivatives of this class of compounds show fluorescence because of the double bond hindering, which occurs due to cyclization.[18]

Several characterization techniques in collaboration with computational chemistry help in recognizing the applied aspects of a known or unknown compound. In the context of theoretical validation of experimental results, the density functional theory (DFT) represents increasingly useful tool in dealing with a diversified size and nature of molecules.[22,23] Metal nitrosyl complexes have also been investigated thoroughly using DFT and other machine-learning tools to explore various parameters of applied interest.[24] There has been great indistinctness for the use of functionals and basis sets corresponding to such type of study. The use of various functionals and basis sets with respect to nitrosyl complexes to seek the chemical nature of NO.[25,26]

In connection with the interest toward the formulation of Ru(II) nitrosyls complexes, this work describes DFT-experimental combinatory evaluation of a new

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