



A novel tetrahedral silver complex of (z)-o-methyl s-hydrogen tosylcarbonimidothioate: DFT supported crystallographic and spectroscopic study

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ARTICLE INFO

Keywords:

Silver
Tosyl
DFT
Spectroscopy
Tetrahedral

ABSTRACT

This article aims to discuss the synthesis and DFT-experimental formulation of a tetrahedral silver complex of (z)-o-methyl s-hydrogen tosylcarbonimidothioate. Spectroscopic and other analytical data reveal that the ligand behaves as monobasic unidentate ligand and reacts with Ag(I) core in 1:1 ratio to give diamagnetic complex of the general composition [Ag(L)(PPh₃)₃], where LH denotes the ligand. The complex has been characterized using FT-IR, UV-Visible, mass spectral analyses and single X-ray crystallography in addition to other preliminary non-instrumental techniques. Also, the optimized framework of the proposed geometry has been confirmed from DFT calculations at LANL2DZ/B3LYP level of theory. The vibrational frequencies of the complex the corresponding normal modes were evaluated at the optimized geometry using the same basis sets followed by other required spectroscopic computation. From the results it is evident that the complex bears tetrahedral geometry with the tosyl ligand binding through S-anionic site.

1. Introduction

Silver is one of the most important metals having prominent medicinal and other industrial values [1–4]. The compounds of this metal are effective antimicrobial agents [5,6] anti-inflammatory candidates [7], and are also used in the form of recommended chemotherapeutics [8–10]. In the meantime synthesis of silver complexes [11] is not only to develop potential drug molecules but to also find the applicability in homogenous catalysis to prepare new compounds involving C–C and C–N bond activation [12]. Due to the fact of possessing high biocidal activity against microbes, silver complexes are suggested as agents of multitude applications for agricultural purposes in addition to other sectors [13–15]. Ultimately the biological features along with other applied aspects including structural orientation of a metallic compound depends on the nature of a ligand and the nature of central metal [16–19]. In the prevailing coronaviral pandemic the entire scientific world is trying to develop a permanent treatment for this deadly disease

[20]. Due to these increasing infections thus there is an urgent requirement to carry out the investigations on new effective agents [21, 22]. Under such a fascination Silver complexes of carbene have emerged as satisfactory antimicrobial compounds [23–26].

In conspicuous fascination towards the complexes of silver and also, due to the growing applied interest towards C–S bond activation mediated by metal [27–29], this work describes the synthesis and characterization of (Z)-O-methyl S-hydrogen tosylcarbonimidothioate based Silver complex. Scheme 1 displays the dianionic ligand that was used in this work, providing enhanced charge delocalization, and the presence of both the hard and soft donor sites in the form of N, O and S. This makes such type of complexation different in terms of electronic and structural details [30–33]. Moreover, the incorporation of phosphines as co-ligands is expected to create dramatic modification in physico-chemical properties of the resulting complex [34]. The complex has been characterized by several techniques including DFT supported X-ray crystallography.

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<https://doi.org/10.1016/j.jics.2022.100626>

Received 21 May 2022; Received in revised form 30 June 2022; Accepted 30 June 2022

Available online 3 July 2022

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