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# DMSO coordinated dioxidomolybdenum(VI) complexes chelated with 3-methoxybenzhydrazone related ligands: Synthesis, structural studies and *in vitro* cytotoxicity

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ABSTRACT

Three new DMSO coordinated dioxidomolybdenum(VI) complexes $[MoO_2L^{3OMe}(DMSO)]$ (**1**), $[MoO_2L^{4OMe}(DMSO)]$ (**2**) and $[MoO_2L^{5OMe}(DMSO)]$ (**3**) (where, $L^{3OMe}$ = 2-oxy-3-methoxybenzaldehyde-3-methoxy-benzhydrazonato, $L^{4OMe}$ = 2-oxy-4-methoxybenzaldehyde-3-methoxybenzhydrazonato and $L^{5OMe}$ = 2-oxy-5-methoxybenzaldehyde-3-methoxybenzhydrazonato) (Scheme 1) were synthesized by reacting $[MoO_2(acac)_2]$ with the corresponding aroylhydrazone in presence of the solvent, DMSO and fully characterized. The various characterization techniques included elemental analysis, spectroscopic techniques (IR, electronic and $^1$H NMR), thermogravimetric analysis and cyclic voltammetry. The molecular and crystal structures of **1**, **2** and **3** were determined by single crystal X-ray diffraction method. In all complexes, the molybdenum atom displays a distorted octahedral geometry. In addition, the discussion on coordination geometries and non-covalent interactions were also supported using Hirshfeld surface analysis. The *in vitro* cytotoxicity of the aroylhydrazone ligands and their molybdenum complexes against lymphoma ascites cell line demonstrated that the complexes are more cytotoxic than their corresponding ligands.



## 1. Introduction

Aroylhydrazones characterized by azomethine group (RC═N—) are excellent multidendate ligands that form a significant class of compounds in medicinal and pharmaceutical chemistry and are known to have biological applications due to their antibacterial [1–6], antifungal [3–6] and antitumor [7,8] activities. Moreover the incorporation of transition metals into these compounds [9] can lead to the enhancement of their biological property [10,11]. As one of the versatile element of the periodic table, spanning oxidation states of −2 to +6, molybdenum has drawn the attention of the coordination chemist in general [12–16]. At the present moment, the coordination chemistry of molybdenum has become a prospective area of research due to the significant enzymatic role played by molybdenum in biochemical reactions [17–19] especially in the oxidation of aldehydes, purines and sulfides [20].

In this context, the oxidomolybdenum complexes coordinated with tridendate ligands have drawn significant attention due to their similarity to the active site of majority of molybdoenzymes [12,21]. This enzymatic role of molybdenum in biological reactions has created a tremendous impetus in the syntheses of a number of model complexes mimicking oxotransferase molybdoenzymes [13,22–27]. Molybdenum(VI) Schiff base complexes with a *cis*-$MoO_2$ core are excellent enzyme model systems for this purpose. Moreover possessing an Mo═O unit has been widely used in catalysis for numerous industrially important chemical reactions such as hydrogen generation [28], alkene epoxidation [29,30] and sulfide oxidation [31].

In spite of the synthesis of many molybdenum Schiff base complexes, there are few reports on the cytotoxicity of these complexes, though our group have reported the synthesis and *in vitro* cytotoxicity studies of dioxidomolybdenum(VI) complexes derived from an ONO donor aroylhydrazone with different donor auxilliary ligands [32]. In continuation of our previous study [32], the present study focuses on the effect of position of the methoxy substituent on the aldehydic part (keeping the hydrazide part constant) on their crystal structures and *in vitro*-cytotoxicity.

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