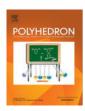
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# DMSO coordinated dioxidomolybdenum(VI) complexes chelated with 3-methoxybenzhydrazone related ligands: Synthesis, structural studies and *in vitro* cytotoxicity



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#### ABSTRACT

Three new DMSO coordinated dioxidomolybdenum(VI) complexes [MoO<sub>2</sub>L<sup>3OMe</sup>(DMSO)] (1), [MoO<sub>2</sub>L<sup>4OMe</sup>(DMSO)] (2) and [MoO<sub>2</sub>L<sup>5OMe</sup>(DMSO)] (3) (where, L<sup>3OMe</sup> = 2-oxy-3-methoxybenzaldehyde-3-methoxy-benzhydrazonato, L<sup>4OMe</sup> = 2-oxy-4-methoxybenzaldehyde-3-methoxybenzhydrazonato and L<sup>5OMe</sup> = 2-oxy-5-methoxybenzaldehyde-3-methoxybenzhydrazonato) (Scheme 1) were synthesized by reacting [MoO<sub>2</sub>(acac)<sub>2</sub>] 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.

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### 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<sub>2</sub> 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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