



# Synthesis, structural insights and catalytic activity of a dioxidomolybdenum(VI) complex chelated with N<sup>4</sup>-(3-methoxyphenyl) thiosemicarbazone

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## Abstract

A *cis*-dioxidomolybdenum(VI) complex of a thiosemicarbazone of the type [MoO<sub>2</sub>L(DMSO)], where H<sub>2</sub>L = 3-ethoxysalicylaldehyde-N<sup>4</sup>-(3-methoxyphenyl) thiosemicarbazone was synthesized. The molecular structure was determined by SCXRD analysis. The complex crystallizes in triclinic *P* $\bar{1}$  space group. The structure consists of a distorted octahedral geometry around central metal, molybdenum. The various hydrogen bonding and  $\pi \cdots \pi$  interactions were explored. Further, the nature and importance of these interactions in the crystal packing were revealed with the help of Hirshfeld surface analysis. Moreover, the synthesized compounds were characterized by physicochemical and spectroscopic methods. Redox properties of the compounds were analyzed by cyclic voltammetry. Finally, the molybdenum complex was evaluated for its catalytic potential for the oxidation of styrene and it displayed about 97% product selectivity for the oxidation of styrene to styrene oxide.

## Introduction

Thiosemicarbazones serve as excellent multidentate ligands that can coordinate with most of the transition metals forming complexes with varied structural features [1–4]. Similarly *cis*-dioxidomolybdenum(VI) complexes chelated with tridentate ONS donor ligands are of great importance in the domain of coordination chemistry owing to their ability to serve as model systems for the active site of the molybdoenzymes such as xanthine oxidase and sulfite oxidase [5, 6]. Moreover, the molybdenum complexes of thiosemicarbazones show excellent catalytic capacity related to the structural features of the coordinated *cis*-MoO<sub>2</sub> unit, chelate ring structure and also substituents on the ligands [7, 8]. In addition to that, some of the molybdenum complexes also

catalyze oxygen atom transfer reactions [9, 10]. With the exception as being models of enzymatic active sites, molybdenum complexes of tridentate thiosemicarbazone ligands are important because of their potential catalytic activity [11, 12].

Herein, we report the synthesis and spectral characterization of a dioxidomolybdenum(VI) complex [MoO<sub>2</sub>L(DMSO)] of a thiosemicarbazone ligand, H<sub>2</sub>L reported by us [13], and having appropriate structure to catalyze oxidation as well as oxo-transfer reactions. The complex contains doubly deprotonated tridentate form of 3-ethoxysalicylaldehyde-4-(3-methoxy)phenyl thiosemicarbazone (H<sub>2</sub>L) and was characterized using elemental analysis, FTIR, UV–Vis and <sup>1</sup>H NMR spectroscopies. The crystal structure was solved by single-crystal X-ray diffraction technique. To end with, the catalytic potential of the complex was investigated for the oxidation of styrene.

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## Experimental

### General remarks

The starting materials, 3-ethoxy-2-hydroxybenzaldehyde, N<sup>4</sup>-(3-methoxyphenyl) thiosemicarbazide and bis(acetylacetonato) dioxidomolybdenum(VI) metal precursor were supplied by Sigma-Aldrich chemical company.