

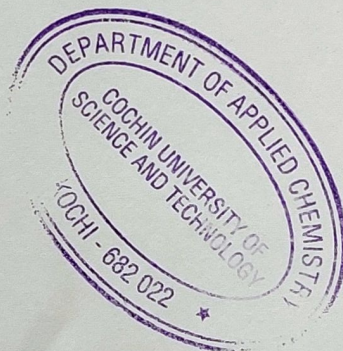
23/03/2023

**CERTIFICATE**

This is to certify that Dr. Nithya Mohan, Assistant Professor, Basic Science and Humanities department, SCMS School of Engineering and Technology is associated with one of my project "Salen Schiff base complexes: Synthesis and applications" from 01/11/2022.

Dr. P.V. Mohanan

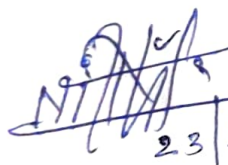
Professor



## Work Report of the collaborative work


### Third order NLO studies on Schiff base complexes with aliphatic diamine spacer groups

We have synthesized novel symmetrical salen schiff base complexes and the third order linear and nonlinear optical properties were studied. The experimental results revealed that the synthesized compounds are good NLO active materials and the third order nonlinear property arises from two photon absorption (TPA). Materials having such two photon absorption (TPA) have wide range of application in the field of optical storage memory, photodynamic therapy<sup>1</sup> etc. The optical limiting values show that the reported compounds are good optical limiters. The experimental results were substantiated with theoretical calculations carried out using DFT at B3LYP/6-31G\* level of theory. The system with the highest  $\pi$ -delocalisation exhibited the highest activity. The total dipole moment, polarizability and first hyperpolarizability were also calculated at the same level of theory which are also in line with the experimentally observed results.



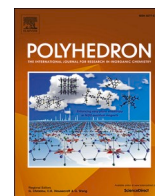
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# Mononuclear and binuclear dioxidomolybdenum(VI) chelates derived from a tridentate ONO donor aroylhydrazone: Spectral, structural, DFT and *in silico* biological investigations

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## ABSTRACT

Four dioxidomolybdenum(VI) complexes,  $[\text{MoO}_2(\text{L})]_2 \cdot \text{H}_2\text{O}$  (1),  $[\text{MoO}_2(\text{L})(\text{py})]$  (2),  $[\text{MoO}_2(\text{L})(3\text{-pic})] \cdot \text{H}_2\text{O}$  (3) and  $[\text{MoO}_2(\text{L})(4\text{-pic})]$  (4) of a dibasic tridentate ONO donor aroylhydrazone,  $\text{H}_2\text{L}$  (where  $\text{H}_2\text{L}$  = 3-methoxy-2-hydroxybenzaldehyde-2-furoic acid hydrazone) have been synthesized and well characterized. The stoichiometric reaction of aroylhydrazone with  $\text{MoO}_2(\text{acac})_2$  in methanolic medium yielded phenoxobridged binuclear complex 1 whereas monomeric complexes, 2, 3 and 4 were formed as a result of incorporating different monodentate heterocyclic bases. The tridentate aroylhydrazone coordinates to the  $\text{MoO}_2^{2+}$  core through phenolate oxygen, azomethine nitrogen and iminolate oxygen atoms. Single crystal XRD studies established the coordination geometry of mononuclear dioxidomolybdenum(VI) complexes as distorted octahedron. The crystal structures and various solid state interactions were also investigated here. DFT investigations were conducted to explore the reactivity parameters of the studied aroylhydrazone and complexes. Furthermore, molecular docking analyses unveiled the superior putative binding energy of the investigated compounds in contrast to cisplatin. These findings were particularly pronounced in relation to the selected target proteins, which are indicative of their potential efficacy against lung and breast cancer cell lines.

## 1. Introduction

Aroylhydrazones encompassing multiple donor sites in the structural framework proves to be one of the potential ligand systems and these compounds along with their transition metal complexes have attracted the researchers due to their multifaceted applications [1–9]. Among the different transition metal complexes derived from aroylhydrazones, the design and synthesis of dioxidomolybdenum(VI) complexes of aroylhydrazone with dibasic tridentate ligand system containing accessible coordination sites are especially significant on account of its applications in substrate binding reactions [10–12]. The ability to promote facile electron-transfer pathways and ligand exchange reactions enhanced the versatility of molybdenum as a biometal [10–12]. Apart from the diverse molecular architectures rendered by the molybdenum (VI) complexes [13–16], they also function as efficient catalytic

materials in oxotransferase reactions [17], industrially relevant reactions [18,19] as well as an excellent model for molybdoenzymes [20].

In preceding publications, we detailed the synthesis and intricate structural characterization of dioxidomolybdenum(VI) complexes featuring aroylhydrazone ligands whose sixth labile coordination site was found to be engaged either by diverse solvents, encompassing water, DMF or DMSO [21–25] or bidentate heterocyclic base like 4,4'-bipyridine [21]. It is found that the heterocyclic base, 4,4'-bipyridine coordinated dioxidomolybdenum(VI) complex can be a suitable candidate for substrate binding reactions due to the large and weak  $\text{Mo}-\text{N}_{\text{base}}$  bond as an outcome of the *trans* effect of oxo oxygen atom of *cis*- $\text{MoO}_2^{2+}$  core which is evident from XRD studies [21]. The introduction of heterocyclic base as coligands into metal ions also found to increase the hydrophobicity of the complexes in turn enhancing the biological activity [6,26]. These results stimulated our interest and encouraged us to

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