



Spectral studies and crystal structures of molybdenum(VI) complexes containing pyridine or picoline as auxiliary ligands: interaction energy calculations and free radical scavenging studies

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Abstract

Three *cis*-MoO₂ complexes [MoO₂(CAB)(py)] (**1**), [MoO₂(CAB)(3-pic)] (**2**) and [MoO₂(CAB)(4-pic)] (**3**) which vary in the nature of the heterocyclic bases in the auxiliary coordination site derived from an ONO donor aroylhydrazone (H₂CAB) have been synthesized and characterized by various physicochemical methods. The single-crystal X-ray diffraction studies reveal that the complexes adopt a distorted octahedral N₂O₄ coordination sphere around the Mo(VI) center in which the ONO donor atoms of hydrazone moiety and one oxido oxygen constitute the NO₃ basal plane and the axial position by the other oxido oxygen and nitrogen atom of coordinated pyridine molecule in [MoO₂(CAB)(py)] (**1**) or picoline molecule in [MoO₂(CAB)(3-pic)] (**2**) and [MoO₂(CAB)(4-pic)] (**3**). The hydrogen bonding interaction generates a two-dimensional supramolecular sheet-like architecture in [MoO₂(CAB)(py)] (**1**) and [MoO₂(CAB)(3-pic)] (**2**), whereas a three-dimensional network was observed in [MoO₂(CAB)(4-pic)] (**3**). The interaction energy calculations reveal that the dispersion energy component dominates over other components and [MoO₂(CAB)(3-pic)] (**2**) is found to be energetically more stable. Furthermore, the aroylhydrazone shows free radical scavenging activity, whereas the complexes are inactive.

Introduction

Aroylhydrazones are well-established class of molecules with several possible structures including configurational isomers, viz. *E* and *Z*, around the imine (C=N) bond and amido/iminol tautomers. Due to the presence of multiple donor sites such as protonated/deprotonated amide oxygen, imine nitrogen and additional donor site (usually N or O) provided from the carbonyl compound, they exhibit diverse chelating modes with greater effects in a wide variety of fields [1–4]. The presence of the azomethine group (–NH–N=CH–) connected with carbonyl group makes them

responsible for different biological activities, such as anti-oxidant, anti-inflammatory, anti-hypertensive, antimicrobial and anticancer properties [5–10]. Among transition metals, the chemistry of molybdenum has become an important area due to its potential application in diverse fields [11–15]. Molybdenum complexes have a unique place in the advancement of coordination chemistry [16]. Due to their extended applicability in biology and pharmacology, complexes containing pyridine ring moieties are of great interest [17–20]. The field of supramolecular architecture is very important in coordination chemistry. Various supramolecular interactions including conventional and non-conventional hydrogen bonds and non-covalent interactions such as π – π interactions, C–H \cdots π , anion (halide) \cdots π and even C–H \cdots C interactions gave rise to a number of 1D, 2D and 3D supramolecular architectures [21–23].

Due to their facile synthesis, structural flexibility, stability and high potential as efficient catalysts, a great deal of work has been carried out on the synthesis and characterization of *cis*-dioxidomolybdenum(VI) complexes containing the [MoO₂]²⁺ core [24–26]. The articles regarding the biological activities of molybdenum complexes are, however, much more limited. The present study reports the syntheses, spectral and structural characterization of *cis*-MoO₂

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