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Research paper

Supramolecular frameworks formed via hydrogen bonding and non-covalent interactions and interaction energy calculations of solvent coordinated *cis*-dioxomolybdenum(VI) complexes derived from ONO donor aroylhydrazone: Cytotoxicity studies

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ABSTRACT

A tridentate ONO donor aroylhydrazone, 3,5-diiodosalicylaldehyde-4-methoxybenzoylhydrazone (H_2SMB) and four *cis*-MoO_2 complexes [MoO_2(SMB)(DMF)] (**1**), [MoO_2(SMB)(DMSO)] (**2**), [MoO_2(SMB)(py)] (**3**) and [MoO_2(SMB)(3-pic)] (**4**) which vary the solvents/heterocyclic bases in the sixth coordination position have been synthesised. The compounds were characterized by different physico-chemical methods. The single crystal X-ray diffraction studies unambiguously confirm the molecular structures. In the complexes **1, 2, 3** and **4,** the octahedral geometry around the Mo(VI) central atom is satisfied by ONO donor atoms and two oxo oxygens, the sixth coordination site is occupied by oxygen/nitrogen atoms of solvent molecules. The supramolecular architectures generated by various hydrogen bonding and non-bonding interactions were investigated. The interaction energy calculations reveal dominance of dispersion energy component over other components. The aroylhydrazone was screened for antioxidant study using DPPH assay. The *in vitro* cytotoxicity of Mo(VI) complexes was evaluated against lymphoma ascites cell line as well as against normal cell and compared to hydrazone and cyclophosphamide.

1. Introduction

Hydrazones constitute a well-established class of proligands and are easily synthesized by condensing hydrazines with carbonyl compounds. They can coordinate to metal ions *via* azomethine N atom and the substituent donor groups through various chelating modes [1–4]. Hydrazones display a wide range of applications in the field of biology. The increased biological activities allow hydrazones to occupy pre-eminent position in the area of medicinal chemistry. Hydrazones have the ability to show various biological activities like antioxidant, anti-inflammatory, antidiabetic, anticonvulsant, analgesic, antimicrobial, antitumour, anti-HIV *etc* [5–13]. The biological properties of hydrazones might be altered significantly upon complexation with transition metal ions.

Metal complexes containing supramolecular architecture are very important in coordination chemistry. The non-covalent interactions form the basis for the design of supramolecular architecture leading to complicated crystal packing and greater attention has given to the study of variety of these interactions. The prevailing supramolecular interaction is classical O/N—H···O/N hydrogen bonds (interaction energy 16–60 kJ mol^{-1}) followed by O/N—H···halide hydrogen bonds. The C—H···O/N hydrogen bonds (16 kJ mol^{-1}), non-covalent interactions including π···π interactions (< 2–20 kJ mol^{-1}), C—H···π (4–10 kJ mol^{-1}), (halide-) anion···π and even C—H···C interactions constitute weaker control forces [14–24]. It is also well documented that non-covalent interactions form the backbone of the molecular aggregates [25–27]. Hydrazones have the ability to form complexes with most of the transition metals. Among transition metals, the research in the field of molybdenum complexes has gained greater attention than ever before. The molybdenum related research can be categorised into molybdenum complexes showing catalytic activities, interesting structural patterns relevant to active sites of various molybdoenzymes etc [28–30]. Though Mo(VI) is relatively harmless to the environment, applications of molybdenum complexes in the field of biology are much limited.

In literature, although the antitumour activity of hydrazone

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