



A Schiff base colorimetric chemosensor for CN⁻ ion and its dioxidomolybdenum (VI) complexes: Evaluation of structural aspects and optoelectronic properties

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Six new *cis*-dioxidomolybdenum(VI) complexes featured with a tridentate ONO donor Schiff base derived from salicylidene-2-aminophenolato backbone have been synthesised and characterised by elemental analysis, spectroscopic techniques (like IR, UV-vis and ¹H-NMR) and cyclic voltammetry. Suitable single crystals of the parent complex [MoO₂L(MeOH)]₂·H₂O (**1**) was obtained by the slow evaporation of the mother liquor, whereas the crystals of the complexes **2-6** were grown in coordinating solvents like ethanol, DMF, DMSO *etc.* and were characterised by single crystal X-ray diffraction as monomers stabilised by the solvent molecules used for the recrystallization purpose. The structures of the complexes were further quantified using Hirshfeld surface analysis. The Schiff base acts as a colorimetric chemosensor for CN⁻ ions in DMSO solution. The receptor-CN⁻ ion interaction and the sensing mechanism of the chemosensor were verified by colorimetric, UV-vis, ¹H-NMR and FT-IR spectroscopic studies. Hydroxyl moiety present in the receptor function as the binding site for cyanide ion thereby leading to its optical discrimination in presence of other anions by producing a visible colour change from colourless to yellow. Therefore the Schiff base sensor portrays estimable selectivity and sensitivity towards CN⁻ ion. Additionally the Schiff base as well as the molybdenum complexes exhibit good third order non-linear optical properties and optical power limiting when analysed by the Z-scan technique.

KEYWORDS

cyanide ion, Hirshfeld surface analysis, molybdenum complexes, non-linear optical property, Schiff base, Z-scan technique

1 | INTRODUCTION

Anions show a decisive role in biology, specifically in the metabolism of all living organisms, medical field, environmental science, chemical and industrial processes.^[1] Nevertheless these anions are vital for living

organisms, unnecessary accumulation of these anions in human body leads to the perpetual damaging effect to the various organs including kidney, bones, liver^[2] *etc.* Amongst the various anions, cyanide ion is the most fretful one since it plays a death-defying role as a pollutant in environmental as well as biological field.^[3]