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# ACCEPTED MANUSCRIPT

## Mononuclear oxovanadium(IV) Schiff base complex: Synthesis, spectroscopy, electrochemistry, DFT calculation and catalytic activity.

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### **Abstract**

A new complex of oxovanadium, VOL has been synthesized from Schiff base ligand obtained by the condensation of *o*-phenylenediamine and 5-bromo-salicylaldehyde. All new compounds have been characterized by <sup>1</sup>H NMR, IR spectra, UV-Vis spectroscopy, elemental analysis and mass spectrometry. The molar conductance data revealed that the metal complex is a non-electrolyte. Thermal analysis techniques (TGA/DTA) of the ligand and the complex were performed. The proposed structures for the free ligand and the corresponding vanadium complex were corroborated by the use of geometry optimization and conformational analysis. The solid state structure of complex VOL was fully determined by single crystal X-ray diffraction analysis.

Similar electrochemical behavior for both the ligand and the corresponding complex have been observed by cyclic voltammetry (CV). The complex gave a metal-based one-electron quasi-reversible redox couple at 606 mV/SCE corresponding to the VO<sup>IV</sup>/VO<sup>V</sup> redox process which was consistent with the hydrodynamic voltammograms. Additional peaks in the CVs that were growing with the scan rate have been attributed to consecutive one-electron reduction of the ligand. The catalytic activity of the oxovanadium Schiff base complex VOL was tested in the oxidation reaction of cyclohexene. The efficiency of the catalyst was influenced by the nature of the oxidant. The results showed that the complex was highly active and selective for cyclohexenone in optimized conditions.

**Keywords:** Oxovanadium complex, Synthesis, Spectroscopy, Crystallography, DFT, Cyclic Voltammetry, Oxidation.

### **1. Introduction**

In recent decades Schiff bases play an important role in inorganic chemistry as they easily form stable complexes with most transition metal ions [1-3]. The coordination chemistry of

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