

Tolyldithiophosphates of Vanadium: Synthesis, Characterization, Antimicrobial, Cytotoxic and DFT Studies

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Abstract:

*New complexes of vanadium(III) corresponding to $[(ArO)_2PS_2]_3V$ and $[(ArO)_2PS_2]_2VCl.L$ (Ar = o-, m-, p-CH₃C₆H₄ and p-Cl-m-CH₃C₆H₃; L = NC₅H₅, P(C₆H₅)₃, have been synthesized and characterized by various physico-chemical techniques like elemental analyses, magnetic studies, mass, IR, UV and NMR (¹H, ¹³C and ³¹P) spectral studies. The presence of a six coordinated vanadium atom has been established in the complexes and adducts, respectively. The ligands and the complexes have been optimized using density functional theory (DFT). The structural parameters, vibrational bands and energy gaps of frontier orbitals (HOMO–LUMO) have been calculated. The calculated geometric and spectral results reproduced the experimental data with well agreement. Theoretical calculated frontier molecular orbitals (HOMO–LUMO) and their energies suggest charge transfer occurs within the complexes. Antimicrobial screening of the complexes against two bacterial strains: Gram–positive, *Enterococcus faecalis* and Gram–negative, *Escherichia coli* and fungus *Fusarium oxysporum* have shown potential bioactivity. The cytotoxic analysis was carried out using the cultivated human cell lines: lung adeno carcinoma cell line A-549, leukemia cell line THP-1, prostate cancer cell line PC3 and colorectal cancer cell line HCT-116.*

Keywords Vanadium •Dithiophosphate •Phosphorus •Sulfur •Antimicrobial