

Synthesis and characterization of low-nuclearity oxidovanadium(IV) complexes with biologically relevant molecules

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Many oxidovanadium complexes have been explored for their potential medical applications, mainly as antimicrobial, anticancer, and antidiabetic drugs¹. Recently, our research group reported that the antibacterial activity of decavanadate anion is improved when combined with biologically relevant molecules, such as vitamin B3². Aiming to expand the number of compounds evaluated, the reactivity of 3-pyridinecarboxamide, 3-pca, and well-known oxidovanadium anions, generated *in situ* were explored. The reaction of V₂O₅, oxalic acid and 3-pca (1:3:3) in an aqueous solution at 60 °C, generated a blue solid (Product 1) in good yield and a few amounts of green crystals (Product 2), after the addition of propane-2-ol. The IR spectra of both compounds showed expected bands at 980-985, 1656-1680, 3350-3097 cm⁻¹ assigned to $\nu(\text{V}=\text{O})$, $\nu(\text{C}=\text{O})$ and $\nu(\text{N}-\text{H})$, respectively. Product 1, was characterized as (3-pcaH)₂[VO(OH₂)(C₂O₄)₂](μ -C₂O₄) by elemental analysis (Anal. calcd. for C₁₈H₁₈N₄O₁₈V₂ (%): C, 31.8; H, 2.66; N, 8.24, V, 14.9. Found: C, 31.9; H, 2.86; N, 8.38; V, 14.5), thermogravimetric analysis and by infrared (IR), electron paramagnetic resonance (EPR) and electronic spectroscopies. EPR spectra of 1 present only a broad line centered at $g = 1.981$, characteristic of binuclear vanadium(IV) complexes ($I = 7/2$), confirming the reduction of the vanadium(V) to (IV). The microcrystalline nature of 1 was indicated by powder X-ray diffraction. Product 2, in turn, crystallizes in orthorhombic system, *Pna*2₁ space group, and consists of the mononuclear complex (3-pcaH)₂[VO(C₂O₄)₂], with two bidentate oxalate ligands and differs from the other analogues described in the literature³ by the combination with two 3-pcaH⁺ cations. Herein, two novel oxidovanadium(IV) complexes are being described.

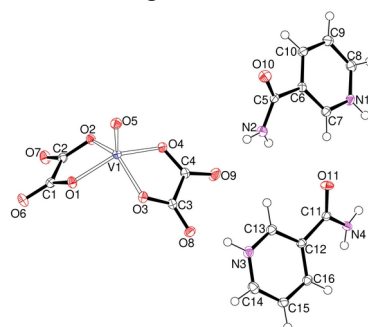


Figure 1. ORTEP diagram of (3-pcaH)₂[VO(C₂O₄)₂], with thermal ellipsoids at 50% probability.

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