

**Название публикации:**

New oxidovanadium(IV) complex with a BIAN ligand: synthesis, structure, redox properties and catalytic activity

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**Аннотация:**

Reaction of  $\text{VOCl}_3$  with bis[N-(2,6-diisopropylphenyl)imino]acenaphthene (dpp-bian) in air afforded  $[\text{VOCl}_2(\text{dpp-bian})]$  (1). The complex was characterized by IR and UV-vis spectroscopies and elemental analysis. The crystal structure of 1 was determined by X-ray diffraction (XRD) analysis. The vanadium atom is in a square-pyramidal  $\text{OCl}_2\text{N}_4$  coordination environment. The cyclic voltammogram (CV) in dichloromethane reveals an irreversible oxidation process at +1.40 V (vs. Ag/AgCl) assigned to the V(IV)/V(V) couple, and two consecutive quasi-reversible one-electron reduction processes at -0.32 V and -1.05 V (vs. Ag/AgCl), respectively, assigned to the bian/bian(-/center dot) and bian(-/center dot)/bian(2-) couples, followed by irreversible reduction at -1.6 V (vs. Ag/AgCl). The EPR spectrum of 1 in toluene shows a single 8-line signal typical for oxidovanadium(IV) complexes with d(1) configuration. The magnetic behavior of 1 confirms the presence of one unpaired electron ( $\mu(\text{eff})$  (330 K) = 1.67  $\mu(\text{B})$ ), and the isolation of the paramagnetic centers. Application of 1 to oxidation of alkanes documented high catalytic activity under mild conditions. The kinetics and selectivity of alkane oxygenation by the 1/ $\text{H}_2\text{O}_2$  and 1/PCA/ $\text{H}_2\text{O}_2$  systems (PCA is pyrazine-2-carboxylic acid) were studied. The reaction is more efficient in the presence of PCA.

**Ключевые слова:**

o-2-h<sub>2</sub>o<sub>2</sub>-vanadium derivative-pyrazine-2-carboxylic acid; diimine ni(ii) catalyst; hydrogen-peroxide; complex-pyrazine-2-carboxylic acid; pyrazine-2-carboxylic acid; vanadium complexes; hydrocarbon oxygenations; pyrazinecarboxylic acid; coordination chemistry; electronic-structure