Structural and magnetic characterization of mixed-valence vanadium (IV/V) complex with $\{(VO)_2(\mu–O)\}^{3+}$ core: Theoretical and experimental insights

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Kolekcja

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Streszczenie

Using deprotonated forms of tetradentate phenol amine ligands 2-((((1-methylbenzimidazol-2-yl)methyl)(pyridin-2-ylmethyl)amino)methyl)phenol (HL^1), dinuclear vanadium(IV,V) complex of composition $[(L^1)_2(V^{IV}O)(\mu\text{-}O)(V^{V}O)](ClO_4)$ (**1**) was synthesized and characterized by X–ray crystallography, UV–Vis, EPR and magnetic susceptibility measurements. Direct current (DC) variable-temperature magnetic susceptibility measurements on polycrystalline sample of **1** were carried out in the temperature range 1.8–300 K. Electron paramagnetic resonance and magnetic studies for **1** demonstrated the complete localization of the single 3d electron on one of vanadium ion and very weak antiferromagnetic interaction between the paramagnetic vanadium(IV) ions in the crystal lattice. The cyclic voltammogram observed with **1**, revealed one oxidation process which is tentatively assigned to $V^{IV}V^{V}/V_2{}^{V}$. $[(L^1)_2(V^{V}O)_2(\mu\text{-}O)](ClO_4)_2$ (**2**·2.5CH_2Cl_2) has been synthesized chemically from **1** and were thoroughly characterized by X–ray crystallography, UV–Vis, ^{51}V NMR and IR measurements.

Słowa kluczowe

Mixed-valence, Vanadium complexes, X-ray diffraction, Magnetic properties, EPR spectroscopy, Redox properties, DFT calculations

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