

Synthesis, characterization and magnetic properties of a dinuclear oxidovanadium(IV) complex : magneto-structural DFT studies on the effects of out-of-plane -OCH₃ angle.

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Streszczenie

A new dinuclear oxidovanadium(IV) complex with a symmetric heptadentate N₄O₃-donor ligand, [V₂(O)₂L(μ-OCH₃)] CH₃OH (1), was synthesized and characterized by elemental analysis, spectroscopic methods (FT-IR, UV-Vis and EPR) and single crystal X-ray analysis, where H₃L is the Schiff base ligand obtained by the condensation of triethylenetetramine and 5-bromosalicylaldehyde. Single crystal X-ray analysis indicated that the vanadium(IV) ions have distorted octahedral geometry and are connected together by phenoxy and methoxy bridging groups. The EPR and magnetic susceptibility measurements show weak V···V antiferromagnetic interactions. The analysis of the magnetic susceptibility data with the Bleaney–Bowers equation gave a value for the magnetic coupling constant of $J = -1.60 \text{ cm}^{-1}$ ($H = -JS_1S_2$). A Broken-Symmetry DFT study also agreed with an intramolecular character of the magnetic coupling giving a comparable value for J and showed an important dependence of the magnetic interaction with the out-of-plane shift of the methyl group of the methoxy bridging group.

Słowa kluczowe

Dinuclear oxidovanadium(IV), magnetic studies, X-ray structures, density functional calculations

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