

# Understanding Electronic Structure and Magnetic Anisotropy of $[V(\text{urea})_6]^{3+}$ Molecule using DFT and First Principle *ab initio* Calculations.

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The electronic structure of a trigonally distorted Vanadium(III) complex<sup>1</sup>,  $[V(\text{urea})_6](\text{ClO}_4)_3$  (**1**), has been studied by applying density functional theory (DFT) and *ab initio* calculations for the estimation of magnetic anisotropy, zero-field splitting and spin ground state derived from the CASSCF and NEVPT2 calculations implemented in ORCA. Raman Spectrum shows broad peaks around 1400–1500  $\text{cm}^{-1}$  which is in good agreement with the experimental reported spectra. UV-visible spectra show three closely spaced broad peaks in the higher energy region at 685.94, 728.00 and 743.13 nm respectively. The spin ground state for **1** was found to be triplet as derived from the NEVPT2 transition energies. CASSCF calculations show zero-field splitting (*D*) 3.21  $\text{cm}^{-1}$  with subtle deviation from the experimental reported values.

## References:

[1]. Re´mi Beaulac, Philip L. W. Tregenna-Piggott, Anne-Laure Barra, Høgni Weihe, Dominique Luneau, and Christian Reber, *Inorg. Chem.* **2006**, 45, 3399-3407.