

SUPPLEMENTARY

Cytotoxic evaluations, spectral characterizations and DFT theoretical calculations of new dioxidovanadium(V) complexesOthman I. Alajrawy¹ , Huda A. Hadi², Roaa S. Awad Al-Luhaibi², Sarah S. Sabar³¹Department of Biology, College of Education, University of Fallujah, Fallujah, Iraq²Ministry of Education, The General Directorate of Education, Ramadi, Anbar, Iraq³Ministry of Health, The General Directorate, Tarmia Hospital, Baghdad, Iraq* Corresponding author: othman_ibraheem2000@yahoo.com; ORCID: <https://orcid.org/0000-0002-3509-6060>

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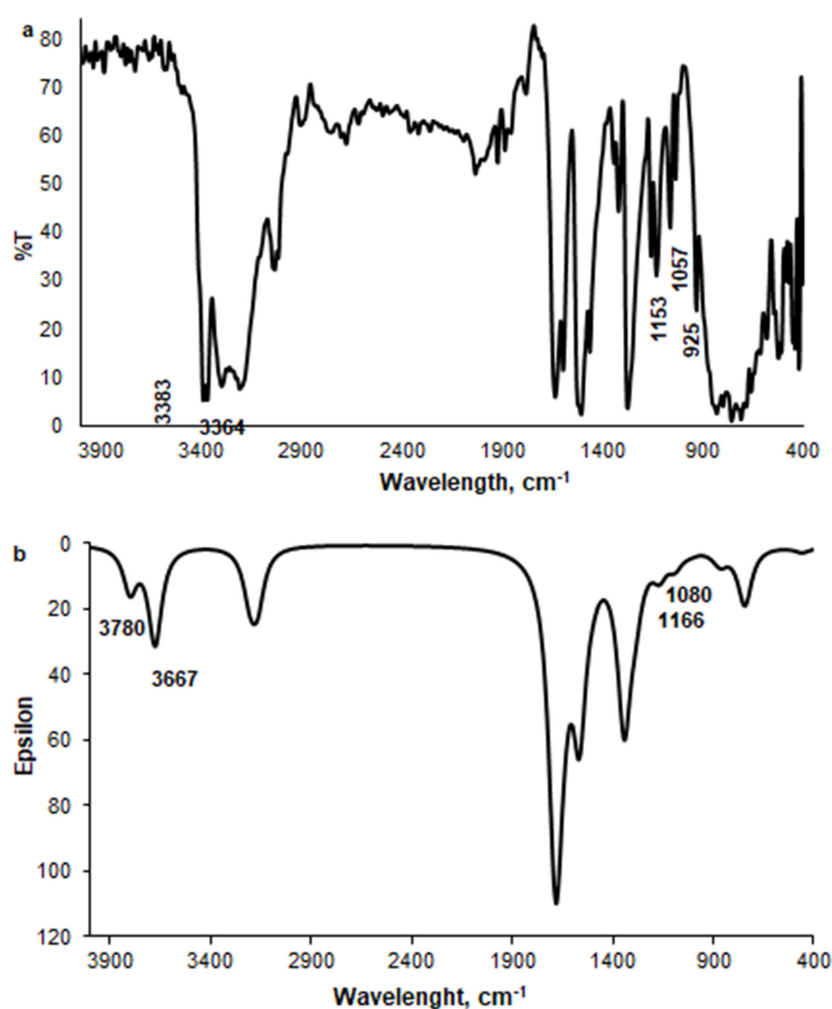


Fig. S1. The FT-IR experimental (a) and calculated (b) spectra of the (OPD) ligand.

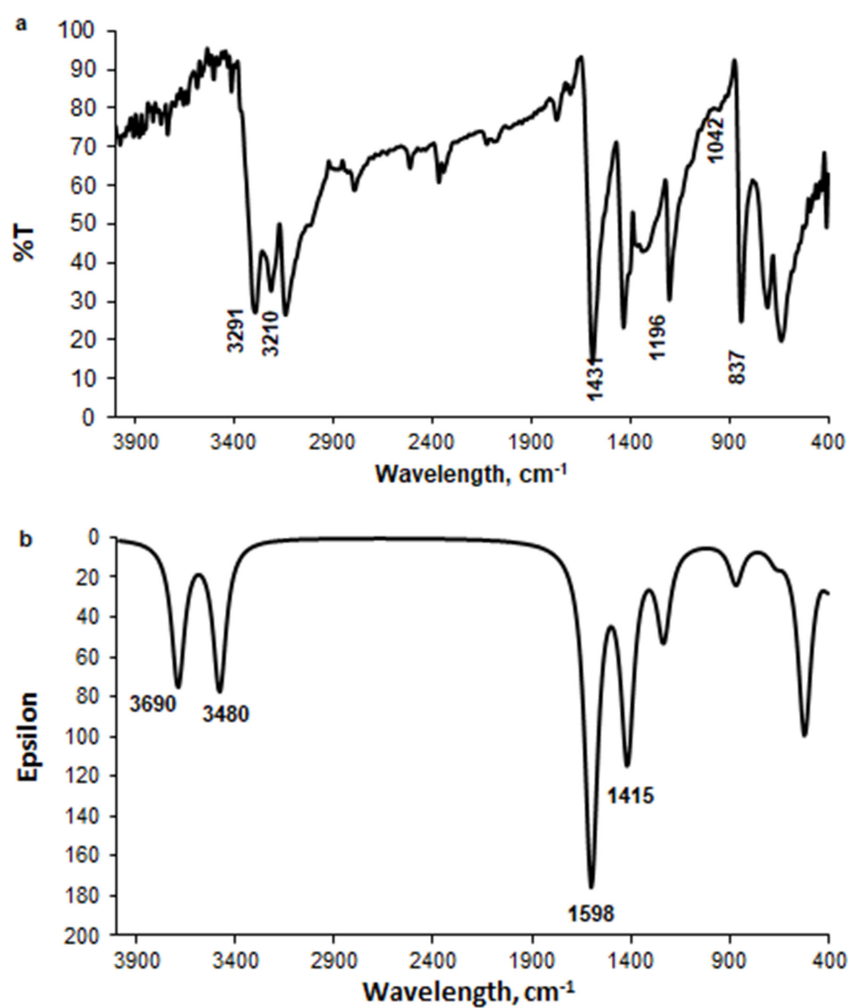


Fig. S2. The FT-IR experimental (a) and calculated (b) spectra of the (DTO) ligand.

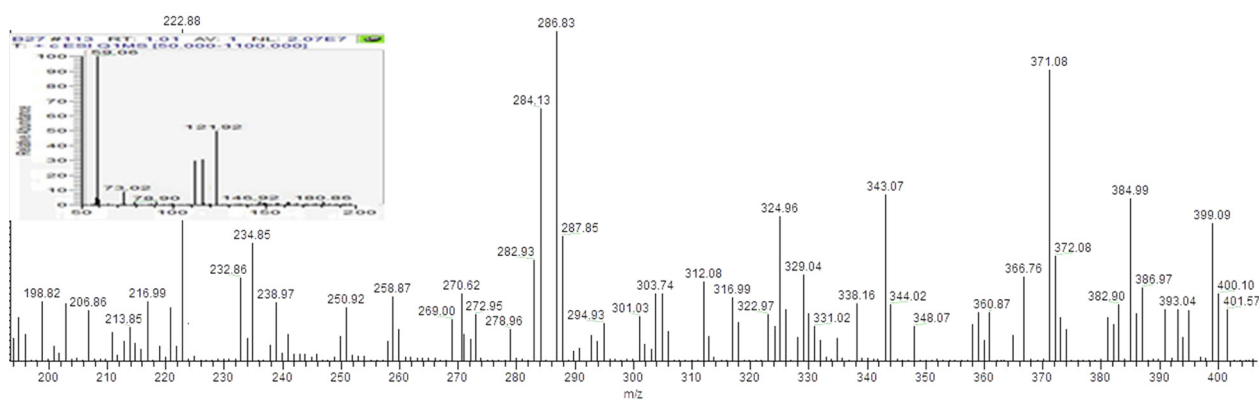


Fig. S3. The mass spectrum of the $[VO_2(OPD)(DTO)]OH \cdot 4H_2O$ complex (2).

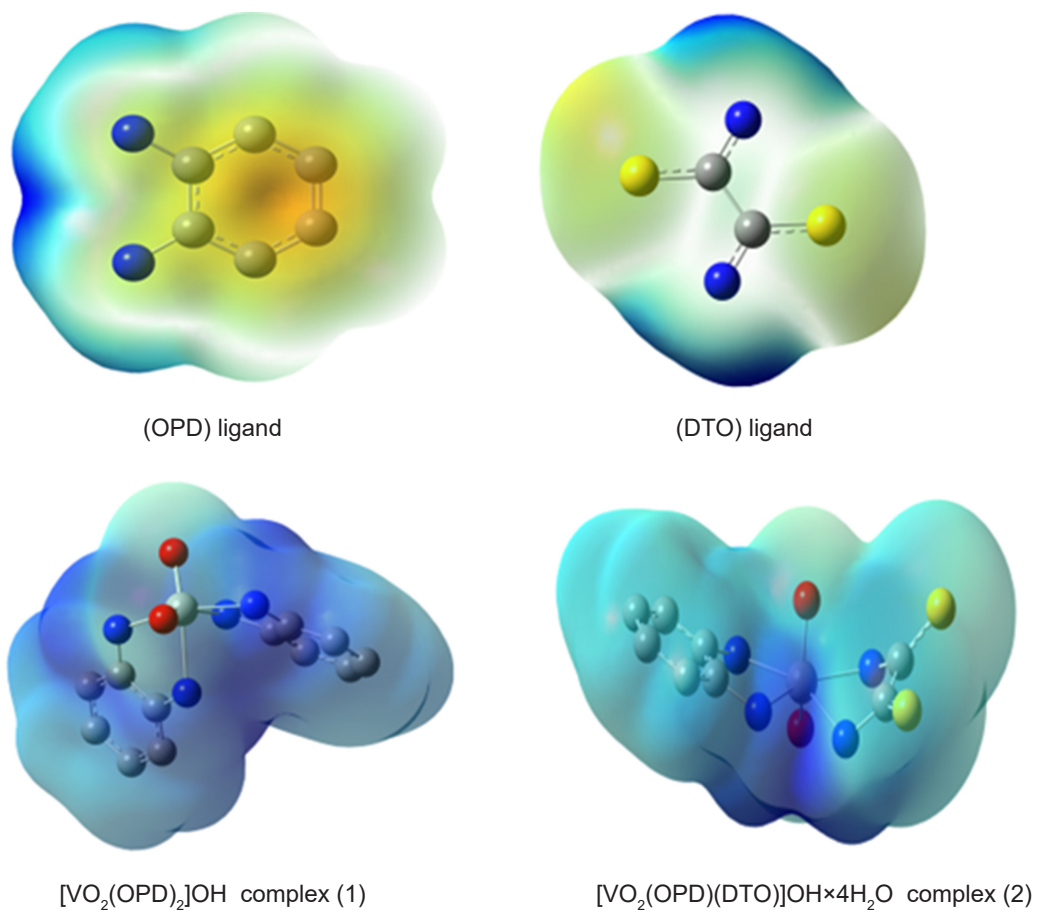


Fig. S4. The (OPD), (DTO) ligands and the dioxidovanadium complexes molecular electrostatic potential (MEP). Vanadium (pale gray), Carbon (deep gray), Nitrogen (blue), Oxygen (red), Sulfur (yellow). The hydrogen atoms were omitted for simplicity.