

Electronic Supporting Information

Journal: Dalton Transactions

Title: Formic acid interaction with uranyl(VI) ion: structural and photochemical characterization

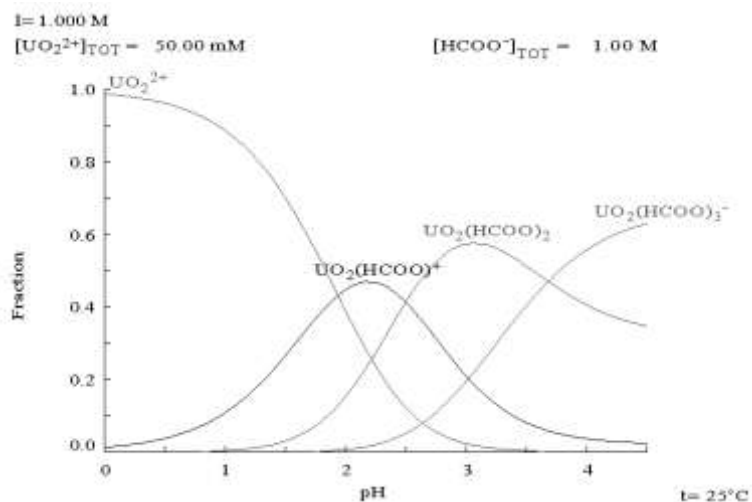


Figure S1 Speciation of the uranyl(VI) formate under present experimental condition using thermodynamic data of Magon, L.; Portanova, R.; Zarli, B.; Bismondo, A.: On the coordination of uranyl(VI) with monocarboxylate anions, *Journal of Inorganic and Nuclear Chemistry* **1972**, 34, 1971-1976. The dataset are for 20°C but the speciation calculation here was performed for 25°C.

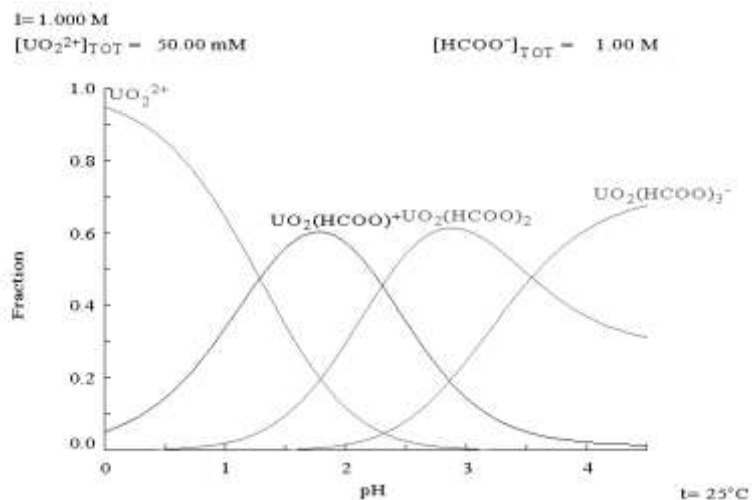


Figure S2 Speciation of the uranyl(VI) formate under present experimental condition using thermodynamic data of Martell, A. E.; Smith, R. M.; Motekaitis, R. J.: *NIST critically selected stability constants of metal complexes database*, Version 5.0, U.S. Department of Commerce, Gaithersburg, MD, U.S.A.

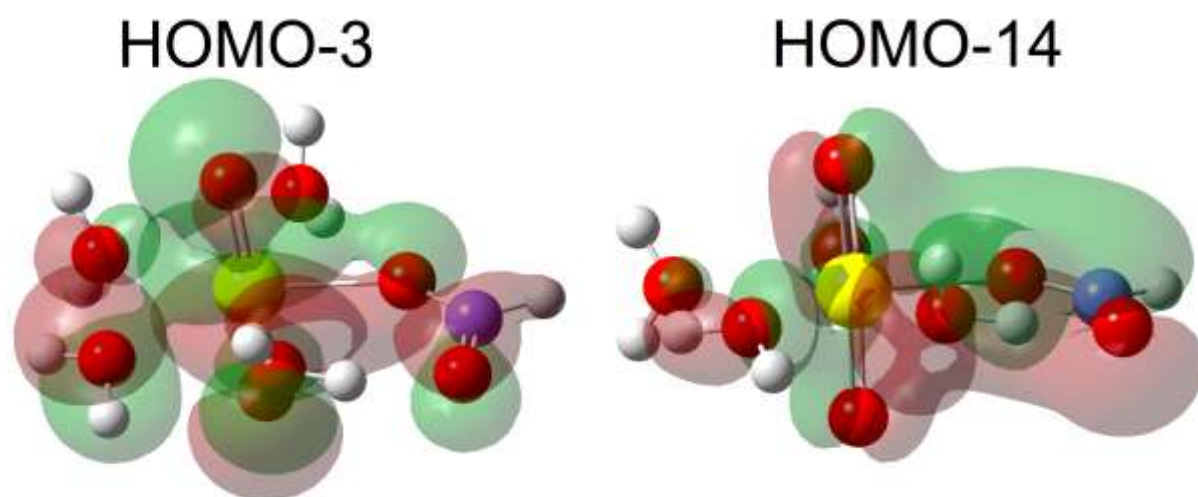


Figure S3 The Kohn-Sham frontier molecular orbitals of uranyl(VI) formate 1:1 uni complex. There are two π interactions between uranyl(VI) and formate in this complex which involve both uranyl σ_u and π_g orbitals.

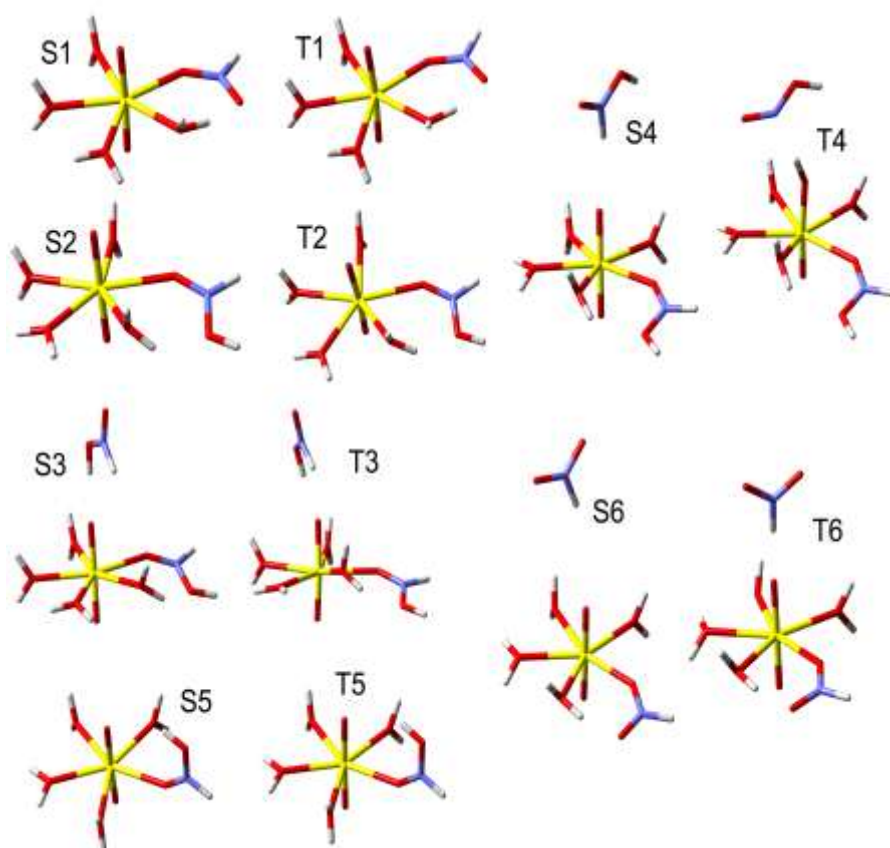


Figure S4 Structures of ground state (**S1–S6**) and lowest-lying triplet state (**T1–T6**) of six models used in this study.