QUANTUM CHEMICAL STUDY ON THE ACTINIDE HYDRATES: THE SOLVENT EFFECTS

T. X. YANG and B.E. BURSTEN, *Department of Chemistry, The Ohio State University, Columbus, OH 43210*; S. TSUSHIMA, *Department of Quantum Engineering and Systems Science, The University of Tokyo, Tokyo 113-8656, Japan*.

Ab initio calculations have been performed to study the structures of the thorium(IV) hydrates, thorium(IV) hydroxide complexes, and curium(III) hydrates in vacuo and in aqueous solution at different levels of theory. The conductor-like polarizable continuum model (CPCM) has been used to conduct geometry optimization computations in aqueous solution. The calculated results demonstrate that the molecular geometries obtained in the solvent generally are consistent with the experiments.