STUDIES ON PLUTONIUM SPECIES

JEAN-PHILIPPE BLAUDEAU[a], BRUCE E. BURSTEN, and RUSSELL M. PITZER, *Department of Chemistry, The Ohio State University, Columbus, OH 43210*.

We will report the status of our ongoing calculations on species containing plutonium. These have had a two-pronged approach: Density Functional Theory Methods (using ADF) studying the speciation of the various plutonium ions in water and multi-reference spin-orbit configuration interaction calculations (using COLUMBUS) studying the electronic structure of plutonyl ions. The speciation studies have concentrated on the comparison of coordination number and Pu-O bond lengths to experimental (from XANES and eXAFS) results. Recently, the electronic structure methods have allowed us to calculate transition spectra. The results for $PuO_2{}^{2+}$ will be reported and compared to experiment.

[a]Present Address: Ohio Supercomputer Center, ASC/MSRC 2435 5^{th} St. B676, Wright-Patterson AFB, Ohio, 45433